Electrostatic and other basic interactions of remote particles

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- electrohydrodynamics (Antonio Ramos, ramos@us.es)
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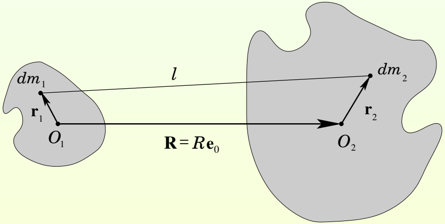
Plan

- Motivation
- Potential energy of pointwise interaction of two remote bodies, general case
- Electrostatic interaction of two remote bodies. Potential energy
- Force and torque acting upon one body from the part of another one depending on their rigid motion
- Additional force and torque due to deformation
- Stress caused by interaction of the bodies

Motivation

- Properties of granular materials depend drastically on their preparation. For instance, when fine grains are fluidized and then are sedimented, they may form aggregates. Formation of aggregates and their interaction depends on their interaction (apart from the interaction with the ambient fluid and the weight of particles). Most of significant interactions have electrical origin (electrostatic and van der Waals forces). For uncharged powders the interaction essentially depends on the distribution of charge due to triboelectricity. Our expressions could be useful for simulation of the aggregation and sedimentation processes and of the behaviour of suspensions.
- Electric interaction between two drops may cause their deformation and motion. For its calculation it is necessary (but not sufficient) to know loads caused by this interaction.
- The true (initial) motivation of this work was a wish to see how torque and force may depend on the relative turn and position of bodies.

Potential interaction of two remote bodies. General case



Pointwise interacting bodies. $d\Pi = f(l)d\mu_1 d\mu_2$.

We suppose that $f(l)$ can be expanded into Taylor series near $l = R$, and $r_i << R$. Note that

$$l^2 = (\mathbf{R} + \mathbf{r}_2 - \mathbf{r}_1) \cdot (\mathbf{R} + \mathbf{r}_2 - \mathbf{r}_1) = R^2(1 - 2h\mathbf{e} \cdot \mathbf{e}_0 + h^2),$$

where $\mathbf{e} = (\mathbf{r}_1 - \mathbf{r}_2)/|\mathbf{r}_1 - \mathbf{r}_2|$, $h = |\mathbf{r}_1 - \mathbf{r}_2|/R = o(1)$.

$$\Pi = \int\limits_{(1)} \int\limits_{(2)} f(R(1 - 2h\mathbf{e} \cdot \mathbf{e}_0 + h^2)^{1/2}) d\mu_1 \, d\mu_2$$

Potential interaction of two remote bodies. General case

We expand the last formula in h. After transformations we have

$$\Pi = \sum_{s=0}^{\infty} \frac{1}{R^s} \sum_{k=0}^{[s/2]} \underbrace{\mathbf{e}_0 \ldots \mathbf{e}_0}_{s-2k} \cdot\!\cdot \ldots \cdot\!\cdot\, F^{(s-k)}(0) 2^{s-k} \sum_{k_1+k_2+k_3=k} \frac{(-1)^{k_3}}{2^{k_1+k_2} k_1! k_2! k_3!}$$

$$\sum_{m=0}^{s-2k} \frac{(-1)^m}{m!(s-2k-m)!} \left(\int\limits_{(1)} r_1^{2k_1} \underbrace{\mathbf{r}_1 \ldots \mathbf{r}_1}_{m+k_3} \, d\mu_1 \cdot\!\cdot \ldots \cdot\!\cdot \int\limits_{(2)} r_2^{2k_2} \underbrace{\mathbf{r}_2 \ldots \mathbf{r}_2}_{s-2k-m+k_3} \, d\mu_2 \right).$$

Characteristics of interaction potential: $F^{(s-k)}(0)$
Distance between bodies centres: R
Direction from one center to another: $\mathbf{e}_0$
Actual distribution of charge/mass in the body: $\int\limits_{(i)} r_i^{2k_i} \mathbf{r}_i \ldots \mathbf{r}_i \, d\mu_i$

Electrostatic interaction of two remote bodies

For electrostatic interaction this yields to

$$\Pi = \frac{k_e q_1 q_2}{R} + \sum_{s=1}^{\infty} \frac{k_e}{R^{s+1}} \sum_{k=0}^{[s/2]} \left(-\frac{1}{2}\right)^k \frac{(2(s-k)-1)!!}{k!(s-2k)!} \sum_{k_1+k_2+k_3=k} \frac{(-2)^{k_3}}{k_1!k_2!k_3!}$$
$$\sum_{m=0}^{s-2k} \frac{(-1)^{s-2k-m}}{m!(s-2k-m)!} \underbrace{\mathbf{e}_0 \ldots \mathbf{e}_0}_{m} \cdot \cdot \ldots \cdot \cdot \int_{(q_1)} r_1^{2k_1} \underbrace{\mathbf{r}_1 \ldots \mathbf{r}_1}_{m+k_3} dq_1$$
$$\cdot \cdot \ldots \cdot \cdot \int_{(q_2)} r_2^{2k_2} \underbrace{\mathbf{r}_2 \ldots \mathbf{r}_2}_{s-2k-m+k_3} dq_2 \cdot \cdot \ldots \cdot \cdot \underbrace{\mathbf{e}_0 \ldots \mathbf{e}_0}_{s-2k-m}.$$

Here $k_e = (4\pi\varepsilon_0\varepsilon)^{-1}$ is the Coulomb constant $(9 \cdot 10^9 N \cdot m^2 C^{-2}/\varepsilon)$.

Electrostatic interaction. First terms of Π

$$
\begin{aligned}
\Pi = & \frac{k_e q_1 q_2}{R} + \frac{k_e}{R^2}\Big(\int \mathbf{r}_1 dq_1 - \int \mathbf{r}_2 dq_2\Big)\cdot \mathbf{e}_0 \\
& + \frac{k_e}{2R^3}\Big(\frac{3}{2}\Big(\int \mathbf{r}_1\mathbf{r}_1 dq_1 + \int \mathbf{r}_2\mathbf{r}_2 dq_2 - 2\int \mathbf{r}_1 dq_1 \int \mathbf{r}_2 dq_2\Big)\cdot\cdot\, \mathbf{e}_0\mathbf{e}_0 \\
& \quad - \int r_1^2 dq_1 - \int r_2^2 dq_2 + 2\int \mathbf{r}_1 dq_1 \cdot \int \mathbf{r}_2 dq_2\Big) \\
& \quad + \frac{k_e}{2R^4}\Big(\frac{5}{6}\Big(\int \mathbf{r}_1\mathbf{r}_1\mathbf{r}_1 dq_1 - \int \mathbf{r}_2\mathbf{r}_2\mathbf{r}_2 dq_2 \\
& \quad + 3\int \mathbf{r}_1 dq_1 \int \mathbf{r}_2\mathbf{r}_2 dq_2 - 3\int \mathbf{r}_2 dq_2 \int \mathbf{r}_1\mathbf{r}_1 dq_1\Big)\cdot\cdot\cdot\, \mathbf{e}_0\mathbf{e}_0\mathbf{e}_0 \\
& \quad + 3\Big(\int r_1^2 dq_1 \int \mathbf{r}_2 dq_2 - \int r_2^2 dq_2 \int \mathbf{r}_1 dq_1 + \int r_2^2 dq_2 \int \mathbf{r}_2 dq_2 \\
& - \int r_1^2 dq_1 \int \mathbf{r}_1 dq_1 - 2\int \mathbf{r}_1 dq_1 \cdot \int \mathbf{r}_2\mathbf{r}_2 dq_2 + 2\int \mathbf{r}_2 dq_2 \cdot \int \mathbf{r}_1\mathbf{r}_1 dq_1\Big)\cdot \mathbf{e}_0\Big) \\
& \qquad + \text{next terms.}
\end{aligned}
$$

Rigid motion and deformation: kinematic relations

Under rigid motion for each body (we omit the body's number 1,2)

$$\mathbf{r} = \mathbf{P}\cdot\mathbf{r}_0, \quad \dot{\mathbf{P}} = \boldsymbol{\omega}\times\mathbf{P}, \quad \dot{\mathbf{r}} = \boldsymbol{\omega}\times\mathbf{P}\cdot\mathbf{r}_0 = \boldsymbol{\omega}\times\mathbf{r} = (\mathbf{r}\times\mathbf{E})\cdot\boldsymbol{\omega}$$

$\mathbf{P}$ is the turn tensor, $\boldsymbol{\omega}$ its angular velocity (both equal for all points of the body).
If the motion is not rigid,

$$\mathbf{r} = \mathbf{f}\cdot\mathbf{r}_0, \quad \mathbf{f} = \mathbf{U}\cdot\mathbf{Q}, \quad \mathbf{U} = \mathbf{U}^s, \quad \mathbf{Q}\cdot\mathbf{Q}^\top = \mathbf{E}, \quad \dot{\mathbf{Q}} = \boldsymbol{\omega}\times\mathbf{Q},$$

where $\mathbf{U}$, $\mathbf{Q}$, $\boldsymbol{\omega}$ may depend on $\mathbf{r}$, and we can obtain

$$\dot{\mathbf{r}} = (\dot{\mathbf{U}}\cdot\mathbf{U}^{-1} + \mathbf{U}\cdot(\boldsymbol{\omega}\times\mathbf{E})\cdot\mathbf{U}^{-1})\cdot\mathbf{r} = \dot{\mathbf{U}}\cdot\mathbf{U}^{-1}\cdot\mathbf{r} - ((\mathbf{U}\times\mathbf{U}^{-1})\cdot\mathbf{r})\cdot\boldsymbol{\omega}$$

For spherical deformation the last term is similar to that of the rigid motion.
If $\mathbf{U}$ is infinitesimal, $\mathbf{U}\cdot\dot{\mathbf{U}}^{-1} \approx (\nabla\mathbf{v})^S$,
$\mathbf{U}\times\mathbf{U}^{-1} \approx \mathbf{E}\times\mathbf{E} - \mathbf{E}\times\nabla\mathbf{u}^S + \nabla\mathbf{u}^S\times\mathbf{E}$, where $\nabla\mathbf{u}$, $\nabla\mathbf{v}$ correspond to the deformation of the body.

Force: not influenced by deformation

$$\dot{\Pi} = -(\mathbf{F}_{21}\cdot\mathbf{V}_1+\mathbf{F}_{12}\cdot\mathbf{V}_2+\mathbf{L}_{21}\cdot\boldsymbol{\omega}_1+\mathbf{L}_{12}\cdot\boldsymbol{\omega}_2) = \mathbf{F}_{21}\cdot\dot{\mathbf{R}}-(\mathbf{L}_{21}\cdot\boldsymbol{\omega}_1+\mathbf{L}_{12}\cdot\boldsymbol{\omega}_2)$$

$$\mathbf{F}_{21} = \sum_{s=0}^{\infty}\sum_{k=0}^{[s/2]} R^{2(k-s)}F^{(s-k)}(0)2^{s-k} \sum_{k_1+k_2+k_3=k} \frac{(-1)^{k_3}}{2^{k_1+k_2}k_1!k_2!k_3!}$$

$$\sum_{m=0}^{s-2k} \frac{(-1)^m}{m!(s-2k-m)!}\left[\bigotimes_{m-1}\mathbf{R}\right] \underbrace{\cdot\cdots\cdot}_{m-1} \int_{(1)} r_1^{2k_1}\left[\bigotimes_{m+k_3}\mathbf{r}_1\right] d\mu_1$$

$$\underbrace{\cdot\cdots\cdot}_{k_3} \int_{(2)} r_2^{2k_2}\left[\bigotimes_{s-2k-m+k_3}\mathbf{r}_2\right] d\mu_2 \underbrace{\cdot\cdots\cdot}_{s-2k-m-1} \left[\bigotimes_{s-2k-m-1}\mathbf{R}\right]$$

$$\cdot\cdot(2(k-s)R^{-2}\mathbf{RRR} + m\mathbf{RE} + (s-2k-m)\mathbf{i}_p\mathbf{R}\mathbf{i}^p)$$

Torque: influenced by deformation

$$\mathbf{L}_{21} = \sum_{s=0}^{\infty} \sum_{k=0}^{[s/2]} R^{2(k-s)} F^{(s-k)}(0) 2^{s-k} \sum_{k_1+k_2+k_3=k} \frac{(-1)^{k_3}}{2^{k_1+k_2} k_1! k_2! k_3!}$$

$$\sum_{m=0}^{s-2k} \frac{(-1)^m}{m!(s-2k-m)!} \Bigg(m\mathbf{R} \times \nabla \mathbf{v_1}^S \cdot \int\limits_{(1)} r_1^{2k_1} \Big[\bigotimes_{m+k_3} \mathbf{r_1} \Big] d\mu_1$$

$$\underbrace{\cdots\cdot}_{k_3} \int\limits_{(2)} r_2^{2k_2} \Big[\bigotimes_{s-2k-m+k_3} \mathbf{r}_2 \Big] d\mu_2 \underbrace{\cdots\cdot}_{s-2k-1} \Big[\bigotimes_{s-2k-1} \mathbf{R} \Big]$$

$$- k_3 \Big[\bigotimes_m \mathbf{R} \Big] \underbrace{\cdots\cdot}_{m} \nabla \mathbf{v_1}^S \cdot \int\limits_{(1)} r_1^{2k_1} \Big[\bigotimes_{m+k_3} \mathbf{r_1} \Big] dm_1 \times \underbrace{\cdots\cdot}_{k_3-1}$$

$$\int\limits_{(2)} r_2^{2k_2} \Big[\bigotimes_{s-2k-m+k_3} \mathbf{r_2} \Big] dm_2 \underbrace{\cdots\cdot}_{s-2k-m} \Big[\bigotimes_{s-2k-m} \mathbf{R} \Big] \Bigg).$$

Stress

We consider the simplest case of homogeneous deformation ($\mathbf{U}$ and $\boldsymbol{\omega}$ do not depend on the point in the body). Then we have (since the pointwise interaction is central)

$$\dot{\Pi} = \mathbf{F}_{21} \cdot \dot{\mathbf{R}} - (\mathbf{L}_{21} \cdot \boldsymbol{\omega}_1 + \mathbf{L}_{12} \cdot \boldsymbol{\omega}_2) + \boldsymbol{\tau}_i \cdot\cdot \nabla \mathbf{v}_i^S$$

As we have obtained before, $\dot{\mathbf{r}}_1 \approx \nabla \mathbf{v}_1^S \cdot \mathbf{r}_1 + \ldots$. Calculating $\dot{\Pi} = \boldsymbol{\tau}_1 \cdot\cdot \nabla \mathbf{v}_1^S + \ldots$, we obtain (omitting the same sums and coefficients that participate in the expression for Π)

$$\boldsymbol{\tau}_1 = \ldots \Bigg(\mathbf{e}_0 \int\limits_{(1)} r_1^{2k_1} \mathbf{r}_1 \ldots \mathbf{r}_1 \, d\mu_1 \cdot\cdot \ldots \cdot\cdot \mathbf{e}_0 \ldots \mathbf{e}_0 \cdot\cdot \ldots \cdot\cdot \int\limits_{(2)} r_2^{2k_2} \mathbf{r}_2 \ldots \mathbf{r}_2 \, d\mu_2$$

$$+ \int\limits_{(1)} r_1^{2k_1} \mathbf{r}_1 \ldots \mathbf{r}_1 \, d\mu_1 \cdot\cdot \ldots \cdot\cdot \mathbf{e}_0 \ldots \mathbf{e}_0 \cdot\cdot \ldots \cdot\cdot \int\limits_{(2)} r_2^{2k_2} \mathbf{r}_2 \ldots \mathbf{r}_2 \, d\mu_2$$

$$+ 2k_1 \int\limits_{(1)} r_1^{2(k_1-1)} \mathbf{r}_1 \mathbf{r}_1 \ldots \mathbf{r}_1 \, d\mu_1 \cdot\cdot \ldots \cdot\cdot \mathbf{e}_0 \ldots \mathbf{e}_0 \cdot\cdot \ldots \cdot\cdot \int\limits_{(2)} r_2^{2k_2} \mathbf{r}_2 \ldots \mathbf{r}_2 \, d\mu_2 \Bigg)$$

Conclusions

- We have calculated the potential energy of a wide class of pointwise interactions of remote particles as an asymptotic series whose terms depend on the characteristics of the charge/mass distribution, distance between the bodies, their turns and displacements
- In particular, of electrostatic, gravitational, van der Waals interaction
- We have calculated also the force, the torque, and the stress for the (rigid motion + homogeneous linear deformation)
- Hopefully it can be useful in simulation of aggregation of triboelectrified and charged powders and behaviour of suspensions or, perhaps, in simulation of formation of celestial bodies

Plans and Acknowledgements

- To find the radius of the convergence of these series
- To think about another approach for close bodies

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I would like to ask all of you who knew Antonio, to write some recollections of him and send me them to elgreco@pdmi.ras.ru.