

Modeling Transport Phenomena of Microparticles
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Lecture – 20
Modeling transport of microparticles – some applications

Hello! Welcome back. So I hope with the previous nineteen lectures you got some idea about the modelling transport phenomena for rigid particles and the viscous drops. And if you recall we discussed in brief similar solutions of stokes equations okay. So it is slightly difficult to follow but today we are going to discuss some applications in particular dealing with the singular representation of stokes flow and then few other applications.

So as I promised when we are discussing the similar solutions I briefly mentioned modelling transport of some microorganisms or particles like motility of sperm etc. So they're very difficult. The reason being is their aspect ratios are very nasty okay. So you have some head like structure and then long tail. So traditional numerical methods do not give okay. So let us see in brief some applications and then maybe how the singular solution can be a very useful tool okay.

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Transport of microparticles and applications

- micro-fluidic environment: flow inside micro-channels/capillaries like arteries, blood flow inside endothelial glycocalyx, mechanical machines
- motility of bacteria, microorganisms, sperm
- viscous drops and bubbles in chemical and bio-reactors

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So typically micro-fluidic environment contains flow inside micro channels capillaries like arteries, blood flow inside endothelial glycocalyx, and some mechanical machines. And other micro particles are like motility of bacterial, micro-organisms and some sperm. And we have discussed viscous drops and bubbles and the lot of applications in chemical and reactors.

So I am sure with the, with this subject when you have done so you can pick up any of the problems ranging from these okay. So followed by the colloid suspensions and electro osmosis etc, right.

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Modeling motility of sperm

Source: Mammalian Sperm Motility: Observation and Theory, E.A. Gaffney, H. Gadelha, D.J. Smith, J.R. Blake, and J.C. Kirkman-Brown. Annu. Rev. Fluid Mech. (2011)

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So one application that I would like to bring to your notice is modelling motility of sperm okay. So the group of John Blake and DJ Smith they have contribute a lot okay. So typically so this is an experiment and this is the simulation. So this is a experiments are in collaboration with the medical community okay. So this is a medical person. So you see the sperms they have a head and then long tail okay. So hence the aspect ratio is very nasty. So if you use any traditional numerical method so you would not get good accuracy okay.

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Modeling cilia beating

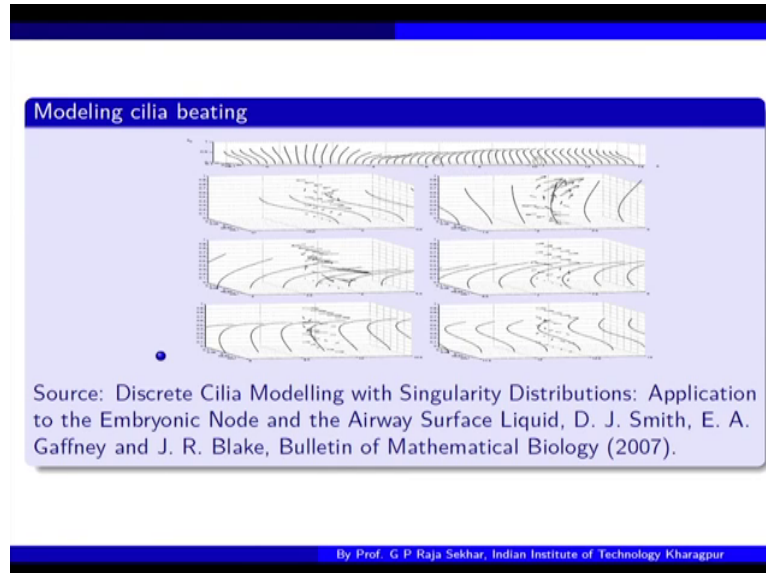
Fig. 2 (A) Cylindrical cilium. (B) Ellipsoidal cilium.

Source: Discrete Cilia Modelling with Singularity Distributions: Application to the Embryonic Node and the Airway Surface Liquid, D. J. Smith, E. A. Gaffney and J. R. Blake, Bulletin of Mathematical Biology (2007).

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And on the other hand so modelling cilia beating okay. So these are like a cylindrical freedom and this is ellipsoidal cilium. And when they are in a fluid so they bend and then collection of cilia produces beating okay. So again from the same group okay. This is a reference.

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So how one would model. So this meta Connell wave has to be modelled. So in order to understand that so individual cilia and then collection of cilia how the corresponding flow field is generated by the cilia has been discussed by the same group okay.

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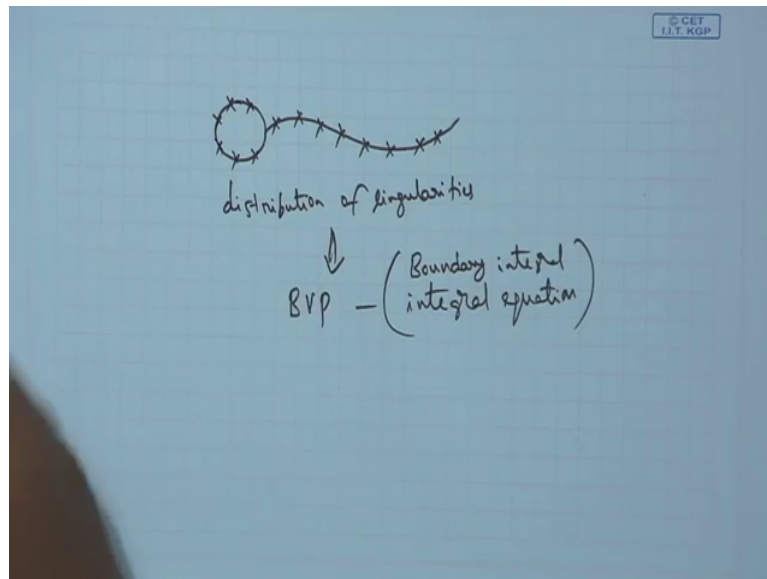
Potential challenges while modeling microparticles

- the aspect ratio do not lead to accurate results using various numerical techniques
- singularity method is best suited

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So now the issue is what are the challenges in modelling such things. As I indicated the aspect ratio do not lead to accurate results using various numerical techniques, therefore, singularity method is best suited okay. So what is the great about the singularity method. So as I mentioned so the technique is as follows.

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You have a head and then longer the details so therefore what happens if you discretize. So this domain is like three dimensions let us say and this is the weather 1D or 2D. So that one has to really get an idea okay. So how one would model this? So as mentioned this is using a singularity method okay. So when you say singularity method what one would do is they distribute singularities okay and then get. So this is distribution of singularities.

Then from here you reduce and obtain boundary value problem which involves which involves an integral equation which typically called boundary integral okay. Of course this is itself is a vast subject. So I am not going into the details but a simple technique of singularities we can discuss. But before that let us see the arbitrary singularity of stokes equation. So let us come to stokes equation.

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Green's function of Stokes Equations

Free space Green's function of Stokes' equations

- Equation of continuity: $\nabla \cdot \mathbf{u} = 0$.
- Stokes equation: $-\nabla P + \mu \nabla^2 \mathbf{u} + \mathbf{g} \delta(\mathbf{x} - \mathbf{x}_0) = 0$, where \mathbf{g} is an arbitrary constant, \mathbf{x}_0 is an arbitrary point

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So we have the corresponding mass conservation and then stokes equation but not the homogeneous one. We are considering a point source on the right hand side with a strength \mathbf{g} . Now we would like to compute the singular solution of this okay. So if you recall in the week 3 we discussed a singular solution of stokes equation but restricted to irrotational. That is due to potential flow.

So now here we would like to discuss the arbitrary singular solution of stokes equation okay. So there are various techniques to solve this but we are showing one of the technique.

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Green's function of Stokes flow

Free space Green's function

- Replace the Dirac delta function as follows $\delta(\hat{\mathbf{x}}) = -\frac{1}{4\pi} \nabla^2 \left(\frac{1}{r} \right)$ where $r = |\hat{\mathbf{x}}|$.
- One can set (obtain) the expression of the pressure as $P = -\frac{1}{4\pi} \mathbf{g} \cdot \nabla \left(\frac{1}{r} \right)$.
- Substituting in the Stokes equation, one may obtain $\mu \nabla^2 \mathbf{u} = -\frac{1}{4\pi} \mathbf{g} \cdot (\nabla \nabla - \mathbf{I} \nabla^2) \left(\frac{1}{r} \right)$.
- Express the velocity in terms of a scalar function H as $\mathbf{u} = \frac{1}{\mu} \mathbf{g} \cdot (\nabla \nabla - \mathbf{I} \nabla^2) H$.

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So replace the Delta function by this. Why? Because we know it. We know Delta function is nothing but. How do we know?

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$$\begin{aligned} \nabla^2 v &= \delta(r) \Rightarrow v(r) = \frac{m}{4\pi} \frac{1}{r} \\ \Rightarrow \delta(r) &= \nabla^2 \left(\frac{1}{r} \right) \frac{m}{4\pi} \\ -\nabla p + \mu \nabla^2 u &= -\bar{g} \nabla^2 \left(\frac{1}{r} \right) \quad (\bar{g} - \text{constant}) \\ -\nabla^2 p &= -\nabla \cdot \frac{\bar{g}}{4\pi} \nabla^2 \left(\frac{1}{r} \right) \Rightarrow \nabla^2 p = \frac{1}{4\pi} \nabla^2 \bar{g} \cdot \nabla \left(\frac{1}{r} \right) \\ \Rightarrow p &= \frac{1}{4\pi} \bar{g} \cdot \nabla \left(\frac{1}{r} \right) + \text{a harmonic function} \end{aligned}$$

Because for Laplacian if you consider delta r we are shown that v is given by some strength by $4\mu \frac{1}{r}$ okay. So therefore what does it mean this means Delta r is Laplacian of one over r of course you can take the corresponding strength okay. So if m is -1 what I have written, we get there. So therefore, we are replacing delta function by this. Then one can one option is you set pressure as this and get the corresponding velocity or we can integrate okay.

So I will show you briefly how we are going to get this okay. So once we have the Stokes equation so this is let us say minus g bar by $4\mu \nabla^2 \frac{1}{r}$. Because what I have done is replace Delta function by the corresponding relation. That is what we have done okay. Then we know that so let us take divergence of that. So divergence of u is 0 so we get from here we get divergence of okay. So now this is a constant. g bar is constant okay.

So from here what we get is $\nabla^2 p = \frac{1}{4\mu} \nabla^2$. So this is I have used a vector identity simply you can use this vector identity. So very straightforward. So this implies p equals $\frac{1}{4}$. So Laplacian and this is also Laplacian okay. Plus a harmonic function. Because any harmonic function can be added. From this we are concluding this right. So therefore, any harmonic function can be added.

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$$0 = -\nabla p + \mu \nabla^2 \bar{u}$$

$$\nabla \cdot \bar{u} = 0 \Rightarrow \nabla^2 p = 0$$

$$p = \frac{1}{4\pi} \int \bar{g} \cdot \nabla' (1/r)$$

$$-\nabla p + \mu \nabla^2 \bar{u} = -\frac{\bar{g}}{4\pi} \nabla^2 (1/r)$$

$$\frac{1}{4\pi} \nabla (\bar{g} \cdot \nabla' (1/r)) + \mu \nabla^2 \bar{u} = -\frac{\bar{g}}{4\pi} \nabla^2 (1/r) = -\frac{\bar{g}}{4\pi} \cdot \mathbf{I} \nabla^2 (1/r)$$

$$\Rightarrow \mu \nabla^2 \bar{u} = -\frac{1}{4\pi} \nabla (\bar{g} \cdot \nabla' (1/r)) - \frac{\bar{g}}{4\pi} \cdot \mathbf{I} \nabla^2 (1/r)$$

But if you see we have for stokes equation, if you combine p is harmonic. So therefore, any harmonic function we are absorbing. So therefore P we are considering it as okay. So that is how we got the pressure. So this is a pressure that I have written okay. So there is a minus sign so maybe we have taken the wrong side. So accordingly we got this. So that is a.

Now corresponding to this P what is the velocity. So that is the next challenge right. So we substitute in the stokes equation okay. So let us do that. This is the P we have. So now we consider the stokes equation which is given by similar stokes equation and we have P. Therefore, we are substituting okay. So this plus Mu okay. So this we have gradient operating here and then we have a Laplacian operating here okay. So we can write this as we can write this as okay.

So this is nothing but the same. I am introducing this is an identity vector okay. So with this we can use okay. So now from here $-\frac{1}{4\pi} \nabla (\bar{g} \cdot \nabla' (1/r))$, we take common. So this term is this then this term so we can use okay. So this what we are doing is this I have taken so this is taken to the other side. So there is a negative sign here and this we have written okay as it is. So there should be okay. So this we have written as it is.

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$$\mu \nabla^2 (\bar{g} \cdot \nabla \nabla - I \nabla^2) H + \frac{1}{4\pi} \nabla (\bar{g} \cdot \nabla (1/r)) = -\frac{\bar{g}}{4\pi} \nabla^2 (1/r)$$

$$\mu \bar{g} \cdot (\nabla \nabla - I \nabla^2) \nabla^2 H = -\bar{g} \cdot (\nabla \nabla - I \nabla^2) (1/r)$$

$$\Rightarrow (\nabla \nabla - I \nabla^2) (\nabla^2 H + \frac{1}{r}) = 0$$

So from here we can adjust. So please note that we are trying to introduce a direct notation which is given by this okay. So this is exactly producing the first term and the second term we are writing as it is okay. So you can verify this is equivalent to this. So where this is a grad on grad okay. So this is called directive notation okay. So from here it is of the form laplacian operating on u equals to some operator on function of r okay.

So this prompts that look for solutions of the form $\bar{u} = \text{some } H$ okay. That means by looking at the structure of this we are looking for solutions of this form okay. So this is similar to let me explain. Suppose we have an operator $L u = \text{let us say we have } r^2 \sin \theta$. So let us call stokes flow past a sphere case a similar structure we have. Then what we are doing we are looking for solutions of the form f of $r \sin \theta$.

So similarly what we are doing. So we have structure of this form so this is the operator on a particular solution. So here the operator is some operator therefore we are taking f okay. So we look for this kind of solution then substitute in the above equation okay. So then what we get is from these two we can conclude so that is what we are doing. Express the velocity in terms of you that means we are looking for this okay.

Then we can substitute in the given equation and observe this will be valid. So how this is a valid? So we are looking for this kind of solution. I am coming back so that there will be μ there okay. So we are looking for such solution. So then we substitute in the stokes equation okay. So once we substitute in the stokes equation we get ∇^2 okay. So this plus so the minus this $-P$ so that is $\text{Grad } P$ okay.

Minus I think P was minus so this is plus this is equal so what is this? This is nothing but. So let me write down. This is Del square u term and this is minus grad p term and this is Delta okay. So once you substitute in this then what we are getting is the following. We get from here so this I am excuse me this is a bracket here okay.

So let me write down this equation in a better form so that we. So this was our u, the format of u. That is what we are seeking the solution. Gradient of p equals the Delta function okay. Now you can commute because we are working in Cartesian and this is a commuting. So from here we get Del square of H. Then these two combining can be expressed in the same operator acting on one over r.

So what we get is $\nabla \cdot \mathbf{g} = -\nabla \cdot \frac{\mathbf{g}}{r}$. Exactly we get this by manipulating the vector identity. So this can be expressed like this okay and this already I have indicated direct notation. And this we have come in okay. So there will be of course μ there okay. So from here what we get is this operator plus 1 over r = 0 okay. So that is what exactly we are showing.

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Green's function of Stokes flow

Free space Green's function

- It will be noted that continuity equation is satisfied for any choice of H .
- $(\nabla \cdot \nabla - \mu \nabla^2) \left(\nabla^2 H + \frac{1}{4\pi r} \right) = 0$.
- The above relation is satisfied if we choose $\nabla^2 H = -\frac{1}{4\pi r}$.
- Integrating twice one may get $H = -\frac{r}{8\pi}$.

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And this above relation satisfies if we choose Del square H equals to -1 over 4 μ r okay. So now this is like we have corresponding Delta function here. So this is the Greens function. So earlier we had the Delta function and then we have solved Del square h = -1 over 4 Pi r okay. So this has to be integrated. So this considering radial symmetry if we integrate we get H

equals to r by 8π okay. So this integration is also very straightforward but maybe corresponding notes will be provided so that you realize right.


So this gives the Green's function of Stokes flow. Which means you have potential flow right but once we have arbitrary flow we can get the arbitrariness Green's function. So the moment H is obtained what is the corresponding velocity we compute.

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Green's function of Stokes flow

Free space Green's function

- We have $\mathbf{u} = \frac{1}{\mu} \mathbf{g} \cdot (\nabla \nabla - I \nabla^2) H$
- $\Rightarrow \mathbf{u} = \frac{1}{\mu} \mathbf{g} \cdot (\nabla \nabla - I \nabla^2) \left(-\frac{r}{8\pi} \right)$
- $\Rightarrow \mathbf{u} = \frac{1}{\mu} \mathbf{g} \cdot (\nabla \nabla) \left(-\frac{r}{8\pi} \right) + \frac{1}{\mu} \mathbf{g} \cdot (I \nabla^2) \left(\frac{r}{8\pi} \right)$
- $\nabla^2 r = \frac{2}{r}$, this gives $\mathbf{u} = \frac{1}{8\pi\mu} \mathbf{g} \cdot [\nabla \nabla (-r) + I \left(\frac{2}{r} \right)]$



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So this is the corresponding velocity. So the H that we have obtained is substituted okay. Then we expand okay so we expand with this then you realize Laplacian operating on r is $2/r$. So therefore, the whole thing can be simplified very much.

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Green's function of Stokes flow

Free space Green's function

- In index notation $u_i = \frac{1}{8\pi\mu} g_j \left(\frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} (-r) + \delta_{ij} \left(\frac{2}{r} \right) \right)$.
- $\Rightarrow u_i = \frac{1}{8\pi\mu} g_j \left(-\left(\frac{r \delta_{ij}}{r^2} - \frac{x_i x_j}{r^3} \right) + \delta_{ij} \frac{2}{r} \right)$
- $\Rightarrow u_i = \frac{1}{8\pi\mu} \left(\frac{\delta_{ij}}{r} + \frac{x_i x_j}{r^3} \right) g_j = \frac{1}{8\pi\mu} G_{ij}(\mathbf{x}, \mathbf{x}_0) g_j$.
- G_{ij} is the free space Green's function of the Stokes equation also referred as Stokeslet or Oseen Burger tensor.



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And in index notation we can write u_i is this. The same expression the same u in index notation we can write okay. Then we simplify this we are operating the derivative on r and then next derivative we are operating on r . So we try to simplify and what we get is finally the free space Green's function of Stokes equation okay. So this is a in a slightly complicated manner but this is a arbitrary solution.

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The image shows a handwritten derivation on a grid background. It starts with the expression for u_i in index notation: $u_i = \frac{1}{8\pi\mu} \left(\frac{\delta_{ij}}{r} + \frac{\hat{x}_i \hat{x}_j}{r^3} \right) g_j$. This is then simplified to $u_i = \frac{1}{8\pi\mu} G_{ij}(\mathbf{x}, \mathbf{x}_0) g_j$, where $G_{ij}(\mathbf{x}, \mathbf{x}_0)$ is underlined and labeled as the 'Stokeslet'. Below this, the tensor G_{ij} is explicitly defined as $G_{ij} = \left(\frac{\delta_{ij}}{r} + \frac{\hat{x}_i \hat{x}_j}{r^3} \right)$. A small logo in the top right corner reads '© CET I.I.T. KGP'.

So what we are getting is. So this in tensor notation typically we write it. So where this denotes the tensor and this particular. So P already we have got okay, so this particular solution is called Stokeslet. Then similar to the potential case if you differentiate the corresponding the higher-order single solutions of Stokes flow can also be obtained okay.

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Green's function of Stokes equation

Free space Green's function

- The vorticity, pressure and the stress fields associated to the flow can be written as

$$\Omega_{ij} = 2\epsilon_{ijl} \frac{\hat{x}_l}{r^3}$$

$$p_i(\hat{\mathbf{x}}) = \frac{2\hat{x}_i}{r^3}$$

$$T_{ijk}(\hat{\mathbf{x}}) = -6 \frac{\hat{x}_i \hat{x}_j \hat{x}_k}{r^5}$$

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So corresponding to the Stokeslet that means if this is the velocity of Stokes flow, then the pressure is given by this stress field is given by this and the vorticity is given by this okay. Now I promised that I will show some application of a singularity method okay. So we will consider correspondingly will consider the corresponding Stokes flow past a sphere that we have done already.

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Application of singularity method

Stokes flow past a solid stationary sphere

Consider a uniform velocity with velocity field \mathbf{U} of an incompressible flow past a solid stationary sphere of radius R . The disturbance flow due to the sphere is represented in terms of a Stokeslet and a potential dipole, both located at the center of the sphere.

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So let us consider that as an okay. So let us consider as an application of singularity method Stokes flow past a solid stationary sphere. So what we are considering? A uniform velocity okay \mathbf{U} and then a sphere of radius R . Our aim is to compute the drag force which is the Stokes drag. Now typically in the separable solution we have shown that we have considered corresponding Stokes stream function and uniform flow added disturbance and computed to the separable solution right.


So here in the singularity method the disturbance will be expanded in terms of singularities okay. So how that is done? The disturbance flow due to the sphere is represented in terms of Stokeslet and a potential dipole. That we have already discussed.

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Stokes flow past a solid stationary sphere

- Consider the following singularity representation:

$$v_i(\mathbf{x}) = U_i + \frac{1}{8\pi\mu} G_{ij}(\mathbf{x}, \mathbf{x}_0) c_j + \frac{1}{4\pi} G_{ij}^D(\mathbf{x}, \mathbf{x}_0) d_j.$$
- \mathbf{c} and \mathbf{d} are the coefficient (strength) of the singularities.
- Explicitly $v_i(\mathbf{x}) = U_i + \frac{1}{8\pi\mu} \left(\frac{\delta_{ij}}{r} + \frac{\hat{x}_i \hat{x}_j}{r^3} \right) c_j + \frac{1}{4\pi} \left(-\frac{\delta_{ij}}{r^3} + \frac{3\hat{x}_i \hat{x}_j}{r^5} \right) d_j$,
 where $r = |\hat{\mathbf{x}}|$, $\hat{\mathbf{x}} = \mathbf{x} - \mathbf{x}_0$.



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Which means we are considering the flow is far field is uniform, then a Stokeslet and a potential dipole okay. So it is slightly the tensor notation etc., slightly difficult but this is just to give you an idea. Now \mathbf{c} and \mathbf{d} are the strengths of the singularity. That means \bar{c} is the strength of the Stokeslet, \bar{d} is the strength of a dipole potential dipole okay. So how do we determine \bar{c} and \bar{d} . Simply you force the no slip condition okay.

So explicit form this is a Stokeslet and this is the potential dipole. We have already considered.

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Stokes flow past a solid stationary sphere

- The boundary condition $\mathbf{v} = \mathbf{0}$ at $r = R$ leads to the following system of algebraic equations:

$$R^2 \mathbf{c} - 2\mu \mathbf{d} = -8\pi\mu R^3 \mathbf{U}$$

$$R^2 \mathbf{c} + 6\mu \mathbf{d} = \mathbf{0}$$

- $\Rightarrow \mathbf{c} = -6\pi\mu R \mathbf{U}$, $\mathbf{d} = \pi R^3 \mathbf{U}$
- Correspondingly, we obtain

$$\mathbf{v}(\mathbf{x}) = \mathbf{U} - \frac{1}{4} \frac{R}{r} \left(3 + \frac{R^2}{r^2} \right) \mathbf{U} - \frac{3}{4} \frac{R}{r} \left(1 - \frac{R^2}{r^2} \right) \frac{\mathbf{U} \cdot \mathbf{xx}}{r^2}.$$

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So now the boundary condition is no slip on the surface of the sphere, so this would be a nice exercise to understand tensor notation and forcing $\mathbf{v} = \mathbf{0}$ on $r = R$. You get these two system of equations. Then one can solve for \mathbf{c} and the \mathbf{d} , which means we have

determined the corresponding velocity field okay. So as you can see this is the corresponding Stokeslet and this is corresponding potential dipoles right.

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Stokes drag

- Traction exerted by the disturbance flow on the sphere is given by $t_i^{dist}(\mathbf{x}) = \frac{1}{8\pi} S_{ijk}^s(\mathbf{x}, \mathbf{x}_0) c_j \eta_k(\mathbf{x}) + \frac{\mu}{4\pi} S_{ijk}^D(\mathbf{x}, \mathbf{x}_0) d_j \eta_k(\mathbf{x}) = \frac{3}{2} \frac{\mu}{R} U_i$.
- Integrating the traction over the surface of the spherical particle, we obtain the hydrodynamic force exerted on the sphere in the form $\mathbf{F} = \int_{Sphere} \mathbf{t} dS = -\mathbf{c} = 6\pi\mu R\mathbf{U}$.

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And corresponding to this the corresponding stress operator on a Stokeslet and the corresponding stress on the potential dipole can be computed and the corresponding stress on the constant is a zero. So therefore if we operate this please recall Week 3 lecture, I have computed the stress of corresponding to potential source. So similarly one can compute the stress corresponding Stokeslet and potential dipole.

So that will be this and one can integrate the stress 3 by $2 R$ by considering the surface element on the sphere. To know the final result will be the Stokes drag okay. So this is a nice application of corresponding Stokes flow past sphere with the singularity method okay. On the other hand there are lots of other applications of micro particles.


For example if you recall thermo capillary migration of a drop that we have discussed. It also has a nice application.

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Droplets in microfluidic devices

- producing calibrated droplets for material science applications
- optimizing the products time-to-market is a major constraint for fine chemicals or pharmaceutical industries
- application of two-phase flow in microchannels: micro droplets as individual nano-volume batch reactors.

Hydrodynamic structures of droplets engineered in rectangular micro-channels, Flavie Sarrazin et. al. Microfluid Nanofluid (2007)



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So we would like to discuss droplets in micro fluidic devices. And the use is producing calibrated droplets for material science applications. So that is a big challenge. For various material science applications you need exactly a droplet of particular size okay. So in order to speed up from the reaction process and to speed up the products to marketing they require micro droplets as individual nano volume batch reactor okay.

So that is very much important application. That means some micro droplets will be used to trigger the reaction. And hence the application of droplet in various channel configurations are very much useful. So these are some literature indicating such phenomena and this is also another literature indicating that phenomena okay.

So these are just to give you some insights about various applications and I hope you get some idea of course understanding the singularity method and the corresponding applications is slightly difficult. But once you spend some time on the tensor notation and understanding singularity of potential flow one can understand singularity methods and then solve some interesting problems okay. Thank you!