

## A note on two boundary integral formulations for particle mobilities in Stokes flow

By SANGTAE KIM<sup>1</sup> AND HENRY POWER<sup>2†</sup>

<sup>1</sup>Department of Chemical Engineering, University of Wisconsin, Madison, WI 53706, USA

<sup>2</sup>Wessex Institute of Technology, Ashurst Lodge, Ashurst, Southampton SO4 2AA, UK

(Received 8 February 1993 and in revised form 14 June 1993)

We show that a recent publication by Liron & Barta (1992) concerning a single-layer boundary integral equation for the tractions is mathematically equivalent to Karrila & Kim's (1989) Riesz method. In actual computational schemes, the second viewpoint is preferable since the integral operator has a spectral radius less than one and even large problems can be solved by fast iterative methods.

The standard boundary integral representation for the Stokes equations for an incompressible Newtonian fluid of viscosity  $\mu$ ,

$$-\nabla p + \mu \nabla^2 \mathbf{v} = 0, \quad \nabla \cdot \mathbf{v} = 0, \quad (1)$$

is 
$$\mathbf{v}(\mathbf{x}) = \frac{-1}{8\pi\mu} \oint_S \mathbf{f}(\boldsymbol{\xi}) \cdot \mathcal{G}(\mathbf{x} - \boldsymbol{\xi}) \, dS(\boldsymbol{\xi}) + \frac{1}{2} \oint_S \mathbf{K}(\mathbf{x}, \boldsymbol{\xi}) \cdot \mathbf{v}_s(\boldsymbol{\xi}) \, dS(\boldsymbol{\xi}), \quad (2)$$

(see Happel & Brenner 1983; Youngren & Acrivos 1975). In the integral representation,  $\mathbf{x}$  is a point of interest in the fluid domain and  $\boldsymbol{\xi}$  is a (dummy) variable for integration over the surface  $S$  that bounds the fluid domain. The surface densities appearing in the two integrals (the integrals are known as the single-layer and double-layer potentials) correspond to surface velocities  $\mathbf{v}_s$  and surface tractions  $\mathbf{f} = \boldsymbol{\sigma} \cdot \mathbf{n}$  for the stress field  $\boldsymbol{\sigma}$ . Our convention for the surface normal  $\mathbf{n}$  is that it points into the fluid domain (so that it points out of the particle in particulate flows). The kernels  $\mathcal{G}$  and  $\mathbf{K}$  are proportional to the fundamental solution of the Stokes equation and its tractions. Explicitly, we have

$$\mathcal{G}_{ij}(\mathbf{x}) = \frac{1}{|\mathbf{x}|} \delta_{ij} + \frac{1}{|\mathbf{x}|^3} x_i x_j, \quad \mathbf{K}(\mathbf{x}, \boldsymbol{\xi}) = \frac{3}{2\pi} \frac{\mathbf{n}(\boldsymbol{\xi}) \cdot (\mathbf{x} - \boldsymbol{\xi})(\mathbf{x} - \boldsymbol{\xi})(\mathbf{x} - \boldsymbol{\xi})}{|\mathbf{x} - \boldsymbol{\xi}|^5}. \quad (3)$$

For disturbance flow fields of a particle submerged in an ambient field  $\mathbf{v}^\infty(\mathbf{x})$ , the double-layer term can be evaluated analytically to yield the simpler equation that uses just a single layer over the particle surface  $S$ ,

$$\mathbf{v}(\mathbf{x}) - \mathbf{v}^\infty(\mathbf{x}) = \frac{-1}{8\pi\mu} \oint_S \mathbf{f}(\boldsymbol{\xi}) \cdot \mathcal{G}(\mathbf{x} - \boldsymbol{\xi}) \, dS(\boldsymbol{\xi}) \quad (\mathbf{x} \in S). \quad (4)$$

We next apply the Newtonian constitutive equation to (4) and evaluate the tractions by dotting with  $\mathbf{n}$ . The result is:

$$\mathbf{f}(\mathbf{x}) + \oint_S \mathbf{K}^*(\mathbf{x}, \boldsymbol{\xi}) \cdot \mathbf{f}(\boldsymbol{\xi}) \, dS(\boldsymbol{\xi}) = 2\mathbf{f}^\infty(\mathbf{x}) \quad (\mathbf{x} \in S), \quad (5)$$

† Permanent address: Instituto de Mecánica de Fluidos, Universidad Central de Venezuela, Caracas, Venezuela.

where the kernel of the adjoint operator is as usual,  $K_{ij}^*(x, \xi) = K_{ji}(\xi, x)$ . Since equation (5) is incomplete (as shown by Odqvist (1930), the null space of  $1 + \mathcal{K}^*$  has dimension six for the single particle problem) Liron & Barta augment it with six auxiliary conditions,

$$\oint_S f_i(\xi) dS(\xi) = F_i, \quad \oint_S (\xi \times f(\xi))_i dS(\xi) = T_i \quad (i = 1, 2, 3), \tag{6}$$

where  $F$  and  $T$  are the hydrodynamic force and torque exerted by the fluid on the particle. It can be shown rigorously that these six conditions are necessary and sufficient to define a unique projection of  $f$  on  $N(1 + \mathcal{K}^*)$  (Power & Miranda 1987).

At first glance, this approach appears to be different from the completed double-layer boundary integral equation of Power & Miranda (1987) and Karrila & Kim (1989) and Karrila, Fuentes & Kim (1989) and this is so claimed in Liron & Barta (1992). Ingber & Mondy (1993) have also made similar comments in their work with a related single-layer representation. However, it can be shown that the Riesz method for extracting the tractions from the completed double-layer representation, first presented by Karrila & Kim (1989), gives a boundary integral equation that is mathematically equivalent to that in Liron & Barta. For the sake of brevity, we omit the mathematical details given in chapter 17 of Kim & Karrila (1991) and go directly to the final result; the completed double-layer boundary integral representation yields

$$f_i(x) + \oint_S \left\{ K_{ij}^*(x, \xi) + \sum_{l=1}^3 \left[ \left( \frac{\delta_{il}}{S^{\frac{1}{2}}} \right) \left( \frac{\delta_{jl}}{S^{\frac{1}{2}}} \right) \right] + \sum_{l=4}^6 \left[ \left( \frac{e_l \cdot (e_{l-3} \times x)}{(I_{l-3})^{\frac{1}{2}}} \right) \left( \frac{e_j \cdot (e_{l-3} \times \xi)}{(I_{l-3})^{\frac{1}{2}}} \right) \right] \right\} f_j(\xi) dS = \frac{1}{S} F_i + \epsilon_{ijk} \left( \frac{T_j}{I_j} \right) x_k$$

as the governing equation for the tractions on a particle moving through a quiescent fluid with known force  $F$  and torque  $T$ . The repeated indices  $j$  imply summation over 1, 2, 3. Also,  $S$  is the surface area of the particle and the  $I_j$  are moments of inertia about the coordinate axes,

$$I_1 = \oint_S (\xi_2^2 + \xi_3^2) dS(\xi), \quad I_2 = \oint_S (\xi_3^2 + \xi_1^2) dS(\xi), \quad I_3 = \oint_S (\xi_1^2 + \xi_2^2) dS(\xi).$$

The sum over  $l$  is shown explicitly to emphasize the structure of the equation, namely

$$f_i(x) + \oint_S \left\{ K_{ij}^*(x, \xi) + \sum_{l=1}^6 [\phi_i^{(l)}(x) \phi_j^{(l)}(\xi)] \right\} f_j(\xi) dS = \frac{1}{S} F_i + \epsilon_{ijk} \left( \frac{T_j}{I_j} \right) x_k. \tag{7}$$

The six vector functions,  $\phi^{(l)}$ , are solutions of  $(1 + \mathcal{K})\phi = 0$ . By direct inspection, we see that these terms correspond to the forces and torques on the right-hand side, by precisely the six auxiliary equations of Liron & Barta. However, equation (7), left as is, is the most efficient way of using the auxiliary conditions because it has Wielandt deflations of the six largest eigenvalues of  $\mathcal{K}$ , an essential step in the iterative solution for very large systems. The deflate-and-iterate scheme maps naturally onto scalable parallel computer architectures as shown in Fuentes & Kim (1992). Given that the auxiliary conditions or the torque are used in a non-trivial fashion, it is unlikely that we would have arrived at this without the mathematical viewpoint of the completed double-layer formulation.

Finally, for the original inhomogeneous problem, equation (5), it is still advantageous to tackle the integral equation with the deflate-and-iterate strategy:

$$f_i + \oint_S \left\{ K_{ij}^* + \sum_{l=1}^6 \phi_j^{(l)} \phi_i^{(l)} \right\} f_j dS = \frac{1}{S} F_i + \epsilon_{ijk} \left( \frac{T_j}{I_j} \right) x_k + 2f_i^\infty.$$

For the important case of multiple particles of arbitrary shape in a bounded domain also of arbitrary shape (e.g. sedimentation of  $M$  particles inside a container), these ideas still apply: the  $6M+1$  auxiliary conditions (the force and torque on  $M$  particles and the no-flux condition through the container surface) can be incorporated as Wielandt deflations of the integral operator. Readers interested in the mathematical details are directed to chapter 17 of Kim & Karrila (1991).

We would like to thank Peyman Pakdel and Douglas Brune (University of Wisconsin), Seppo Karrila (Finnish Pulp and Paper Research Institute), Professor Nadav Liron (The Technion) and three anonymous referees for helpful discussions on this subject.

#### REFERENCES

- FUENTES, Y. O. & KIM, S. 1992 Parallel computational microhydrodynamics: communication scheduling strategies. *AIChE J.* **38**, 1059–1078.
- HAPPEL, J. & BRENNER, H. 1983 *Low Reynolds Number Hydrodynamics*. Martinus Nijhoff.
- INGBER, M. S. & MONDY, L. A. 1993 Direct second kind boundary integral formulation for Stokes flow problems. *Comput. Mech.* **11**, 11–27.
- KARRILA, S. J., FUENTES, Y. O. & KIM, S. 1989 Parallel computational strategies for hydrodynamic interactions between rigid particles of arbitrary shape in a viscous fluid. *J. Rheol.* **33**, 913–947.
- KARRILA, S. J. & KIM, S. 1989 Integral equations of the second kind for Stokes flow: direct solution for physical variables removal of inherent accuracy limitations. *Chem. Engng Commun.* **82**, 123–161.
- KIM, S. & KARRILA, S. J. 1991 *Microhydrodynamics: Principles and Selected Applications*. Butterworth–Heinemann, Boston.
- LIRON, N. & BARTA, E. 1992 Motion of a rigid particle in Stokes flow: a new second-kind boundary integral formulation. *J. Fluid Mech.* **238**, 579–598.
- ODQVIST, F. K. G. 1930 Über die Randwertaufgaben der Hydrodynamik zäher Flüssigkeiten (On the boundary value problems in hydrodynamics of viscous fluids). *Math. Z.* **32**, 329–375.
- POWER, H. & MIRANDA, G. 1987 Second kind integral equation formulation of Stokes' flow past a particle of arbitrary shape. *SIAM J. Appl. Maths* **47**, 689–698.
- YOUNGREN, G. K. & ACRIVOS, A. 1975 Stokes flow past a particle of arbitrary shape: a numerical method of solution. *J. Fluid Mech.* **69**, 377–403.