# Authors' response to Reviewer 1's comments on the submission titled "A spectral boundary integral method for simulating electrohydrodynamic flows in viscous drops"

**by Firouznia, Bryngelson, and Saintillan**

We thank the referee for his/her time and for providing constructive comments on our manuscript. We have carefully addressed all the comments (copied below in black), and the corresponding changes and modifications made in the revised paper are summarized in our response below (in blue). Changes made to the manuscript are also highlighted in blue in the new version.

1. A thorough empirical analysis of convergence and time stepping stability is required for completeness and it will be helpful to future work.

We thank the referee for this suggestion. First, we point out that our original manuscript did include some convergence studies: specifically, Fig. 2 addresses the convergence of the mean curvature calculation, which is an essential component of our method, and Fig. 10 (previously Fig. 8) addresses the convergence of the weighted spherical harmonics method for simulations of low-viscosity drops.

Following the referee's suggestion, we have added a new section to the paper (Sec. 3.6 in the revised manuscript) in which we perform a more thorough convergence analysis for the overall method in the axisymmetric Taylor regime and an analysis of the time step restriction. In Fig. 3(a), we show how our numerical solutions for charge density, velocity field, and drop shape converge to reference solutions on a fine grid with resolution $N^* = 32$ and $M^* = 2N^*$ by plotting the relative errors between these fields as a function of $N$.

For the time step analysis, we calculated the critical time step size for numerical stability using the following bisection method. A model test case is considered with a time horizon of $T = 40$ (in units of $\tau_{\mathrm{MW}}$), such that the system reaches a steady state. Using a relatively large time step size, we perform simulations by marching explicitly in time using a second-order Runge Kutta method. If the simulation is numerically unstable, we divide the time step size in half and repeat the process until we find the maximum time step size required for stability, $\Delta t_c$. Figure 3(b) shows that $\Delta t_c$ varies as $N^{-1}$, which verifies that our CFL condition is first order (see the response to comment 2 below). We observed that increasing the electric capillary number to moderate values $\mathrm{Ca_E} \leq 0.5$ restricts $\Delta t_c$ only by small amounts (less than 3%).

Minor comments:

2. The CFL condition on equation 5 would be $1/N^2$. Any comments on that?

Balancing the convective term with the time derivative in the charge conservation equation

$$\partial_t q + \boldsymbol{n} \cdot [\![ \sigma \boldsymbol{E} ]\!] + \boldsymbol{\nabla}_s \cdot (q\boldsymbol{u}) = 0, \qquad \boldsymbol{x} \in D, \tag{1}$$

shows that the CFL condition is first-order $O(N^{-1})$ in our numerical method. This is verified in Fig. 3(b) of the new manuscript as we discussed in the response to comment 1. Spectral analysis of different operators in our numerical method explains this behavior. We define the single-layer Stokes operator for a vector field $\boldsymbol{f}(\boldsymbol{x})$, $\boldsymbol{x} \in D$ as:

$$\mathcal{S}_D[\boldsymbol{f}](\boldsymbol{x}_0) := \int_D \boldsymbol{G}(\boldsymbol{x}_0;\boldsymbol{x}) \cdot \boldsymbol{f}(\boldsymbol{x})\, \mathrm{d}s(\boldsymbol{x}), \quad \boldsymbol{x}_0 \in D. \tag{2}$$

For simplicity, let's consider the case of $\lambda = 1$ and a spherical drop $D \equiv \mathbb{S}^2$ where the velocity is expressed only in terms of the single-layer Stokes operator (Eq. (25) of the manuscript):

$$\boldsymbol{u} = \alpha\, \mathcal{S}_D[\boldsymbol{f}^H]. \tag{3}$$

$\boldsymbol{f}^{\mathrm{H}}$ is the jump in hydrodynamic traction, and $\alpha = -1/(8\pi\,\mathrm{Ma})$ is a constant. Veerapaneni and coworkers showed that the solution to the Stokes flow equations inside and outside a spherical drop can be expressed as [1]:

$$\boldsymbol{u} = h(r)\boldsymbol{V}_n^m + g(r)\boldsymbol{W}_n^m \tag{4}$$

where $\boldsymbol{V}_n^m$ and $\boldsymbol{W}_n^m$ are the vector spherical harmonics (orthogonal) that are defined in terms of the scalar spherical harmonics $Y_n^m$ and their derivatives as:

$$\boldsymbol{V}_n^m(\theta,\phi) = \boldsymbol{\nabla}_s Y_n^m(\theta,\phi) - (n+1)\, Y_n^m(\theta,\phi)\boldsymbol{n}(\theta,\phi), \tag{5}$$

$$\boldsymbol{W}_n^m(\theta,\phi) = \boldsymbol{\nabla}_s Y_n^m(\theta,\phi) + n\, Y_n^m(\theta,\phi)\boldsymbol{n}(\theta,\phi), \tag{6}$$

$$Y_n^m(\theta,\phi) = \frac{1}{\sqrt{2\pi}} \bar{P}_n^m(\cos\theta)\, e^{im\phi}. \tag{7}$$

$\bar{P}_n^m$ is the normalized associated Legendre polynomial of degree $n$ and order $m$, $m \le n$ (defined by Eq. (28) in the manuscript). Consequently, it can be shown that $\boldsymbol{V}_n^m$ and $\boldsymbol{W}_n^m$ are the eigenfunctions of the Stokes operator defined in (3) (theorem 5.1 in appendix A of [1]):

$$\mathcal{S}_D[\boldsymbol{V}_n^m] = \frac{n}{(2n+1)(2n+3)} \boldsymbol{V}_n^m, \tag{8}$$

$$\mathcal{S}_D[\boldsymbol{W}_n^m] = \frac{n+1}{(2n-1)(2n+1)} \boldsymbol{W}_n^m. \tag{9}$$

The dependence on $(\theta,\phi)$ is suppressed in the notations for simplicity on both sides. Based on (8) and (9), we see that the Stokes operator has a smoothing effect on the spectrum of a target function.

In addition, the surface divergence of $\boldsymbol{V}_n^m$ and $\boldsymbol{W}_n^m$ is given by:

$$\boldsymbol{\nabla}_s \cdot \boldsymbol{V}_n^m = -(n+1)(n+2)\, Y_n^m, \tag{10}$$

$$\boldsymbol{\nabla}_s \cdot \boldsymbol{W}_n^m = -n(n+1)\, Y_n^m. \tag{11}$$

By combining the results of (8) and (9) with (10) and (11), we conclude that the condition number of the charge convection operator grows as $O(N)$ and, therefore, our CFL condition is first-order $O(N^{-1})$ as borne out by our numerical tests.

[1] Veerapaneni, S. K., Rahimian, A., Biros, G., & Zorin, D. (2011). A fast algorithm for simulating vesicle flows in three dimensions. Journal of Computational Physics, 230(14), 5610-5634.

3. An operator split scheme is used between flow and E-field. What are the stability constraints?

Our method uses no operator split scheme. Note that the coupling between the electric field and the flow occurs only through the boundary conditions (Eqs. (5) and (24) of the manuscript). The governing equations for $\boldsymbol{E}$ and $\boldsymbol{u}$ are both time-independent problems. So, at a fixed time, there is only a one-way coupling between these two problems: the dynamic boundary condition (24).

In the first step of the algorithm (presented in Sec. 3), we solve for $[\![E^n(\boldsymbol{x})]\!]$ for a given charge distribution $q(\boldsymbol{x})$ via Eq. (22): this step does not involve the flow. Next, we determine the electric potential $\varphi$ (and $\boldsymbol{E}^{\mathrm{t}} = -\boldsymbol{\nabla}_s\varphi$) through Eq. (20). Having both components of the electric field, we determine the jump in electric reactions $[\![\boldsymbol{f}^{\mathrm{E}}]\!]$ and use it to obtain the hydrodynamic traction $[\![\boldsymbol{f}^{\mathrm{H}}]\!]$ using Eq. (24). Finally, we solve for the velocity field using the Stokes integral equation (25) to obtain the fluid velocity. Once the velocity is known, we calculate the charge density distribution and the drop shape at the next step by time-marching Eq. (5) and advecting the mesh using an explicit RK2 scheme. Therefore, in every step of our algorithm, we solve the exact form of the governing equations for $\boldsymbol{E}$ and $\boldsymbol{u}$ with no alterations.

4. Provide numerical evidence that reparameterization makes a difference

5. Drops appear almost spherical. Are there any examples with more challenging shapes?

We added a test case in Fig. 3 of the revised manuscript corresponding to a drop undergoing large prolate deformations. We showed that the grid quality decreases in the absence of reparametrization, especially near the drop poles where the grid points are depleted over time. This is especially important since the charge concentration is maximum at the poles where the grid has the lowest resolution. Therefore, using reparametrization is essential to obtain an accurate prediction of the overall behavior in this system. We show in Fig. 3 that reparameterization results in a quantitative difference in the predicted drop deformation.

6. In section 3, are you taking just one RK2 step for $q$? Please clarify in the steps

We use a two-step second-order Runge–Kutta scheme to update the charge distribution and drop shape. The corresponding Butcher tableau is

$$\begin{array}{c|cc} 0 & & \\ 1/2 & 1/2 & \\ \hline & 0 & 1 \end{array}$$

To avoid confusion, we modified step 6 of the algorithm provided in Sec. 3 and clarified our time marching method at the end of the paragraph (bottom of page 6).

7. In section 3, what are the time restriction conditions for the time steps. How are the different parameters chosen?

We discussed the restrictions on the time step size in response to comment 1 above, and added some discussion of this in the new Sec. 3.6 of the revised manuscript. For a given resolution $N$, the time step size is chosen to be smaller than the critically stable time step size $\Delta t < \Delta t_c$ discussed in Fig. 4(b). The

grid size $N$ is chosen to ensure convergence of the average deformation $\mathcal{D}$, which was verified to match experimental values and past models in Fig. 6.

Besides the time step size and the number of spherical harmonic modes $N$, all the simulation parameters are material properties and working conditions (i.e., electric field strength). All these parameters, including the electric capillary number $Ca_E$, and Mason number Ma, are determined based on previous works in the literature and are listed in Table 1 of the manuscript. We summarize the reason for selecting each test case in the following:

• System ***S1*** and ***S2*** (Figs. 4-6) are selected as benchmarks since we have experimental measurements [1] as well as simulations [2,3] and small-deformation theories [3-5].

• The Quincke regime was studied for system ***S3*** (Figs. 7, 8), which is selected based on previous experimental [1] and computational studies [2].

• System ***S4*** (Figs. 9, 10) is selected based on the experiments on low viscosity drops by Ouriemi & Vlahovska [6].

• System ***S5*** (Fig. 3) is selected based on previous studies on the dynamics of prolate drops, including [7].

[1] Salipante, P. F., & Vlahovska, P. M. (2010). Electrohydrodynamics of drops in strong uniform dc electric fields. Physics of Fluids, 22(11), 112110.
[2] Das, D., & Saintillan, D. (2017). Electrohydrodynamics of viscous drops in strong electric fields: numerical simulations. Journal of Fluid Mechanics, 829, 127-152.
[3] Das, D., & Saintillan, D. (2017). A nonlinear small-deformation theory for transient droplet electrohydrodynamics. Journal of Fluid Mechanics, 810, 225-253.
[4] Taylor, G. I. (1966). Studies in electrohydrodynamics. I. The circulation produced in a drop by an electric field. Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences, 291(1425), 159-166.
[5] Ajayi, O. O. (1978). A note on Taylor's electrohydrodynamic theory. Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences, 364(1719), 499-507.
[6] Ouriemi, M., & Vlahovska, P. M. (2014). Electrohydrodynamics of particle-covered drops. Journal of fluid mechanics, 751, 106-120.
[7] Lac, E., & Homsy, G. M. (2007). Axisymmetric deformation and stability of a viscous drop in a steady electric field. Journal of Fluid Mechanics, 590, 239-264.

8. I think the sentence above (3) discusses the normal component of $E$ but equation (3) is about the tangential component.

Due to the mismatch in material properties, there will be a jump in the electric field (vector) across the interface along the normal direction, but the magnitude of the jump is unknown. This is discussed in the sentence above Eq. (3). Please note that $\boldsymbol{n} \times [\![ \boldsymbol{E} ]\!] = \boldsymbol{0}$ states that the jump in the electric field vector must be parallel to $\boldsymbol{n}$ (normal vector), and therefore implies that the tangential component is continuous.

9. What are the initial conditions for $q$?

The drop is initially uncharged ($q = 0$) as mentioned in the first paragraph of Sec. 2.1. We emphasized this in the revised manuscript's first paragraph of Sec. 4.

10. Is equation 12 the jump in $f^E$ or just $f^E$? The 11 and 12 seem to use inconsistent notation. Should be 12 be jump$(f^E) = \ldots$

The referee is correct: the left-hand side of Eq. (12) is the jump in electric tractions $[\![ \boldsymbol{f}^{\mathrm{E}} ]\!]$. The typo has been corrected in the revised manuscript.