ACCURACY OF THE COLLOCATION TECHNIQUE

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This document discusses accuracy of the collocation technique we employ to calculate the velocity field in ambient inviscid fluid above an interface swollen by a denser source fluid.

1. Equations

We use notation of our *Physics of Fluids* paper. We define

$$\delta \equiv 1 - B_1', \tag{1}$$

which implies

$$\delta = \sqrt{\frac{1-\zeta}{1+\mathrm{Ri}}}, \tag{2}$$

$$\beta \equiv \frac{gb}{U^2} = \frac{\mathrm{Ri}}{(1+\mathrm{Ri})^{3/2}} \frac{(1-\zeta)^{3/2}}{2\pi\zeta}, \tag{3}$$

with

$$\mathrm{Ri} \equiv \frac{2\pi\zeta\beta}{\delta^3}. \tag{4}$$

The streamfunction in denser source fluid is

$$\hat{\psi}' = -\delta \hat{r} \sin\theta + \theta, \tag{5}$$

yielding the velocity field

$$\hat{u}_r' = \frac{1}{\hat{r}} - \delta\cos\theta, \tag{6}$$

$$\hat{u}_\theta' = \delta\sin\theta. \tag{7}$$

The streamfunction in ambient fluid is

$$\hat{\psi} = -\hat{r}\sin\theta + \theta(1+K_1) + \sum_{n=1}^{N} \frac{F_n}{\hat{r}^n}\sin(n\theta), \tag{8}$$

yielding the velocity field

$$\hat{u}_r = \frac{1}{\hat{r}}(1+K_1) - \cos\theta + \sum_{n=1}^{N} \frac{nF_n}{\hat{r}^{(n+1)}}\cos(n\theta), \tag{9}$$

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$$\hat{u}_\theta = \sin\theta + \sum_{n=1}^{N} \frac{nF_n}{\hat{r}^{(n+1)}} \sin(n\theta). \tag{10}$$

Equation (25) in the PF paper yields

$$(1 + K_1) = \frac{1}{\delta} - \sum_{n=1}^{N} nF_n \delta^n. \tag{11}$$

For collocation, we discretize the interface uniformly into I points as

$$\theta_i = \frac{i\pi}{I+1}, \tag{12}$$

where $i = 1, 2, .., I = N/2$ and N is the number of Eqs. to solve. Note that $\theta = 0$ (stagnation point) and $\theta = \pi$ are both excluded. Radial polar coordinates of collocation points on the interface are

$$\hat{r}_i = \frac{\theta_i}{\delta \sin(\theta_i)}, \tag{13}$$

yielding the elevation

$$\hat{y}_i = \frac{\theta_i}{\delta}. \tag{14}$$

At these points, upon eliminating $\hat{r}_i$ using Eq. (14), the speed squared of source fluid is

$$||\hat{\mathbf{u}}_i'||^2 = \delta^2 \Big[1 + \Big(\frac{\sin\theta_i}{\theta_i} \Big)^2 - 2 \Big(\frac{\sin\theta_i}{\theta_i} \Big) \cos\theta_i \Big], \tag{15}$$

and the speed squared in ambient fluid is

$$\begin{aligned} ||\hat{\mathbf{u}}_i||^2 \quad = \quad & \Big\{ \Big(\frac{\sin\theta_i}{\theta_i} - \cos\theta_i \Big) + \sum_{n=1}^{N} \Big(\frac{\sin\theta_i}{\theta_i} \Big) \Big[\Big(\frac{\sin\theta_i}{\theta_i} \Big)^n \cos(n\theta_i) - 1 \Big] \; nF_n \delta^{n+1} \Big\}^2 \\ + \quad & \Big\{ \sin\theta_i + \sum_{n=1}^{N} \Big(\frac{\sin\theta_i}{\theta_i} \Big)^{n+1} \sin(n\theta_i) \; nF_n \delta^{n+1} \Big\}^2 . \end{aligned} \tag{16}$$

Eliminating β and δ using Eqs. (2)–(4), the system of I Bernoulli's Eqs. at collocation points is

$$\frac{1}{2} \Big[||\hat{\mathbf{u}}_i'||^2 - (1-\zeta) ||\hat{\mathbf{u}}_i||^2 \Big] + (1-\zeta) \frac{\theta_i}{2\pi} \frac{\mathrm{Ri}}{(1+\mathrm{Ri})} = 0, \tag{17}$$

where $||\hat{\mathbf{u}}_i'||^2$ and $||\hat{\mathbf{u}}_i||^2$ are given in Eqs. (15) and (16), respectively. Streamline coincidence at the interface requires that both $\hat{\psi}'$ and $\hat{\psi}$ vanish there. Because Eqs. (5) and (14) already imply $\hat{\psi}' = 0$, coincidence reduces to the system of I Eqs. in ambient fluid:

$$\hat{\psi}_i = \sum_{n=1}^{N} \Big[\Big(\frac{\sin\theta_i}{\theta_i} \Big)^n \sin(n\theta_i) - n\theta_i \Big] \delta^n F_n = 0. \tag{18}$$

Making $\theta_i \to \pi$ in Eq. (18) yields

$$\sum_{n=1}^{N} n\delta^n F_n = 0. \tag{19}$$

Because convergence of the collocation technique is compromised by substituting Eq. (19) into Eqs. (16) and (18), we do not use this relation in our MATLAB implementation of the collocation technique, but instead gauge to what extent Eq. (19) is satisfied after convergence.

Finally, asymptotic slip in the tail is $||\hat{\mathbf{u}}_i|| - |\hat{\mathbf{u}}_i'|| = 1 - \delta$.

2. Linearization

At large N, inspection of Eqs. (12) and (16) reveals that, because $(\delta \sin\theta_I/\theta_I)^N \sim (2\delta/N)^N$ can become very small as $\theta_I = I\pi/(I+1) \to \pi$, increasing $N = 2I$ can raise the last coefficient F_N to much larger magnitude than F_1, and thus make numerical computations stiff and inaccurate. However, if N is not too large, all coefficients in the series can be kept small enough to linearize Eq. (16),

$$||\hat{\mathbf{u}}_i||^2 \simeq \mathbb{B}_i + \mathbb{A}_{in} 2n\delta^{n+1} F_n, \tag{20}$$

with the vector

$$\mathbb{B}_i \equiv 1 + \Big(\frac{\sin\theta_i}{\theta_i}\Big)^2 - 2\Big(\frac{\sin\theta_i}{\theta_i}\Big)\cos\theta_i, \tag{21}$$

and the rectangular matrix of size $I \times N$

$$\begin{aligned} \mathbb{A}_{in} \;\equiv\; & \Big(\frac{\sin\theta_i}{\theta_i} - \cos\theta_i\Big)\Big[\Big(\frac{\sin\theta_i}{\theta_i}\Big)^{n+1}\cos(n\theta_i) - \Big(\frac{\sin\theta_i}{\theta_i}\Big)\Big] \\ + \;& \sin\theta_i \Big(\frac{\sin\theta_i}{\theta_i}\Big)^{n+1}\sin(n\theta_i). \end{aligned} \tag{22}$$

Substitution into I Eqs. (17) yields

$$\mathbb{C}_i \simeq \delta \mathbb{A}_{in}\, \mathbb{F}_n, \tag{23}$$

where

$$\mathbb{C}_i \equiv \frac{1}{2}\Big(\frac{\mathrm{Ri}}{1+\mathrm{Ri}}\Big)\Big[\frac{\theta_i}{\pi} - \mathbb{B}_i\Big] \tag{24}$$

if a vector of size I and

$$\mathbb{F}_n \equiv n\delta^n F_n \tag{25}$$

is a vector of size N to be determined. Similarly, we rewrite the I Eqs. (18) as

$$0 = \mathbb{D}_{in}\mathbb{F}_n, \tag{26}$$

where

$$\mathbb{D}_{in} \equiv \frac{1}{n}\Big(\frac{\sin\theta_i}{\theta_i}\Big)^n \sin(n\theta_i) - \theta_i \tag{27}$$

if a matrix of size $I \times N$. The $N \times N$ linear system of Eqs. to solve for $\mathbb{F}_n$ is then

$$\begin{bmatrix} \mathbb{C}_i \\ 0 \end{bmatrix} = \begin{bmatrix} \delta \mathbb{A}_{in} \\ \mathbb{D}_{in} \end{bmatrix} \Big[\mathbb{F}_n \Big]. \tag{28}$$

3. Errors

Gauge pressure on the interface is

$$p' - p_{\mathrm{atm}} = \rho \frac{U^2}{2} - \rho' \frac{||\hat{\mathbf{u}}'||^2}{2} - (\rho' - \rho) g y, \tag{29}$$

where p_{atm} is atmospheric pressure measured at the altitude y. Meanwhile, the I Bernoulli Eqs. (17) are presented dimensionless with $\rho' U^2$. We evaluate errors in satisfying them relative to stagnation pressure $\rho U^2/2$. We therefore construct a relative error vector for Eqs. (17) by multiplying their residual by $2\rho'/\rho = 2/(1-\zeta)$,

$$\Delta_i \equiv \Big[\frac{||\hat{\mathbf{u}}_i'||^2}{1-\zeta} - ||\hat{\mathbf{u}}_i||^2 \Big] + \frac{\mathrm{Ri}}{(1+\mathrm{Ri})} \frac{\theta_i}{\pi}, \tag{30}$$

for all collocation points $i = 1, 2, .., I$.

To evaluate errors in coincidence of the ambient and source fluid streamlines at the interface, we imagine that the small quantity $\psi_i \neq 0$ represents a source fluid streamline satisfying $\psi' = -\delta R \sin\Theta + \Theta$ that is not quite coincident with the true interface. On that streamline, we locate a point of polar coordinates (R_i, Θ_i) that resides on the normal to the true interface at the collocation point i. We then interpret the distance $\hat{d}_i$ between the two points as a distance error relative to b.

To find $\hat{d}_i$, we first calculate the tangent $\hat{\mathbf{t}}_i$ and normal $\hat{\mathbf{n}}_i$ vectors to the interface at each collocation point,

$$\hat{\mathbf{t}}_i = \frac{1}{\mathbb{B}_i} \Big[\Big(\frac{\sin\theta_i}{\theta_i} - \cos\theta_i \Big) \hat{\mathbf{e}}_r + \sin\theta_i \hat{\mathbf{e}}_\theta \Big], \tag{31}$$

and

$$\hat{\mathbf{n}}_i = \frac{1}{\mathbb{B}_i} \Big[\sin\theta_i \hat{\mathbf{e}}_r - \Big(\frac{\sin\theta_i}{\theta_i} - \cos\theta_i \Big) \hat{\mathbf{e}}_\theta \Big]. \tag{32}$$

We then solve for $\hat{d}_i$ in

$$\hat{\psi}_i = \sum_{n=1}^{N} \Big[\Big(\frac{\sin\theta_i}{\theta_i} \Big)^n \sin(n\theta_i) - n\theta_i \Big] \delta^n F_n = \mathbb{D}_{in} \mathbb{F}_n = \hat{\psi}'(\hat{\mathbf{r}}_i + \hat{d}_i \hat{\mathbf{n}}_i), \tag{33}$$

Equation (5) provides $\hat{\psi}'$ in terms of radial coordinates, $\hat{\psi}'(\hat{\mathbf{r}}_i + \hat{d}_i \hat{\mathbf{n}}_i) = -\delta R_i \sin\Theta_i + \Theta_i$. Cartesian coordinates of the point (R_i, Θ_i) are

$$\hat{X}_i = \Big(\frac{\theta_i}{\delta \tan\theta_i} \Big) + \frac{\hat{d}_i}{\sqrt{\mathbb{B}_i}} \frac{(\sin\theta_i)^2}{\theta_i} \tag{34}$$

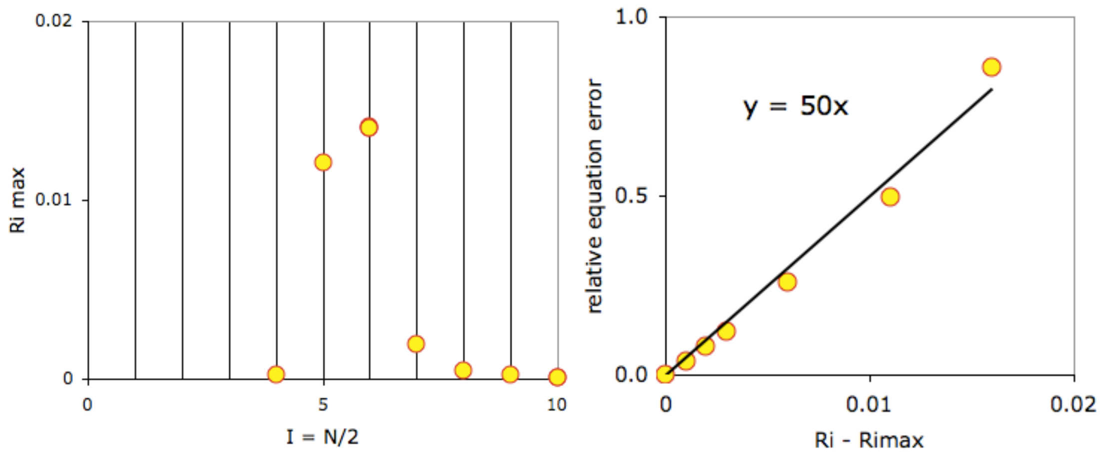

FIGURE 1. Left: $\mathrm{Ri}_{\max}$ vs $I = N/2$, hardly sensitive to ζ. Right: relative error Δ_i vs $\mathrm{Ri}_{\max}$ for $\zeta = 0.1$ and $I = 6$.

and

$$\hat{Y}_i = \frac{\theta_i}{\delta} + \frac{\hat{d}_i}{\sqrt{\mathbb{B}_i}}\Big(1 - \frac{\sin\theta_i\cos\theta_i}{\theta_i}\Big) \tag{35}$$

with $R_i^2 = X_i^2 + Y_i^2$ and $\tan\Theta_i = Y_i/X_i$. Confusing θ_i and Θ_i for simplicity, and treating $\hat{d}_i$ as small, we find

$$\hat{d}_i \simeq -\frac{\psi_i}{\delta}\frac{\sqrt{\mathbb{B}_i}}{(\sin\theta_i)^2}. \tag{36}$$

4. Accuracy

As Fig. 1 shows, at a given $I = N/2$, we find that errors Δ_i and $\hat{d}_i$ are negligible until Ri reaches a maximum value $\mathrm{Ri}_{\max}$ that is a function of I, at which point errors grow linearly with $\mathrm{Ri} - \mathrm{Ri}_{\max}$. Below $\mathrm{Ri}_{\max}$, linearization outlined in section 2 provides a close estimate to the eventual non-linear solution from MATLAB's `fsolve`. $\mathrm{Ri}_{\max}$ is not sensitive to ζ.

Typically, errors Δ_i dominate errors $\hat{d}_i$. Because they can be considerable when $\mathrm{Ri} > \mathrm{Ri}_{\max}$ (Fig. 2), it is unclear whether the non-linear solver has actually found a solution, given that tolerances have to be adjusted until it does.

Note: The MATLAB command for Fig. 2 top was

```
[Fn,err,nFnDeln,th,cur,slip] = DensitySwellingVel(.75,0.27,15,1,0.01,1e-3,10^4,30,1)
```

However, because Cian's simulations have shown that swelling is well captured by the exact theory for source fluid, there is hope that, even if the solver does not predict the ambient velocity field correctly, a solution nonetheless exists.

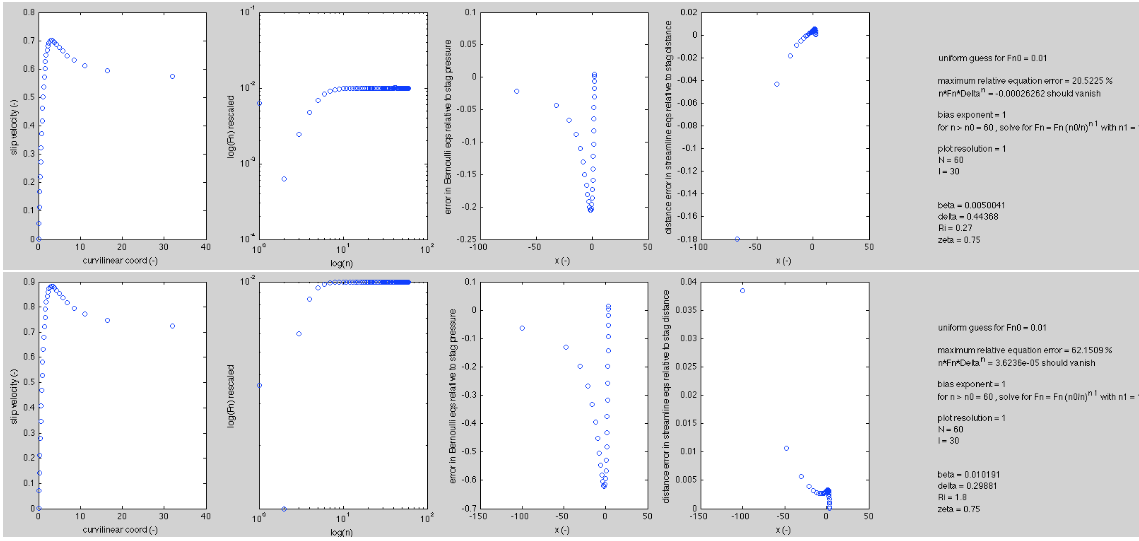

FIGURE 2. Top: MATLAB output with $\mathrm{Ri} = 0.27$, $\zeta = 0.75$ and a tolerance of 10^{-3}, corresponding to the last density point in Fig. (3) of the PF paper; its maximum $\Delta_i \simeq 21\%$. Bottom: for $\mathrm{Ri} = 1.8$, $\zeta = 0.75$ and a tolerance of 10^{-2}, the maximum $\Delta_i \simeq 62\%$.

5. Interface slip

Once all coefficients F_n are known, we calculate interface slip between ambient and source fluids from Eqs. (15) and (16),

$$\frac{u_S - u'_S}{U} = ||\hat{\mathbf{u}}_i|| - ||\hat{\mathbf{u}}'_i||, \tag{37}$$

and we plot this against dimensionless curvilinear distance $\hat{s}' \equiv s/b'$ along the interface, which is independent of δ. We calculate the curvilinear distance by integrating

$$\frac{\mathrm{d}\hat{s}'}{\mathrm{d}\theta} = \frac{1}{\sin\theta}\sqrt{\theta^2 + \left(1 - \frac{\theta}{\tan\theta}\right)^2} \tag{38}$$

use fourth-order Runge-Kutta implemented with `ODE45` in MATLAB. To avoid indeterminacy as $\theta \to 0$, we use $\mathrm{d}\hat{s}'/\mathrm{d}\theta = 1 + 2\theta^2/9 + 14\theta^4/405 + O(\theta^6)$ in that limit.

At or below $\mathrm{Ri}_{\max}$, the slip velocity can be accurately computed for any ζ, as illustrated in Fig. 3

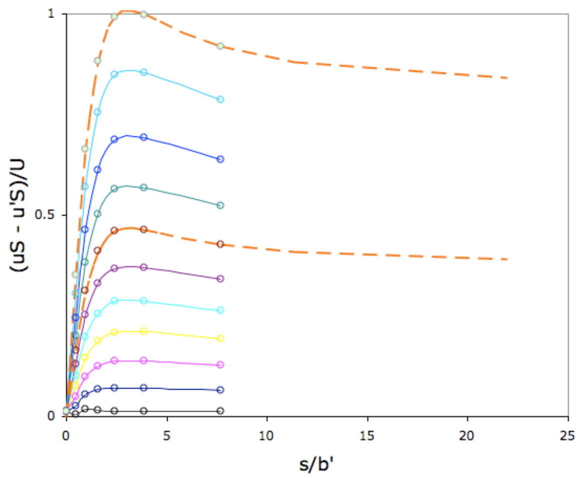

FIGURE 3. Slip velocity $(u_S - u'_S)/U$ at the interface vs $\hat{s}'$ for $\mathrm{Ri} = \mathrm{Ri}_{\mathrm{max}} = 0.014$. Symbols are joined with a curve smoothed by Excel. They are calculated with $I = 6$. From bottom to top: $\zeta = 0.01, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9$ and 0.96. For comparison, the dashed lines are computed with $I = 20$. Despite considerable increase in the magnitudes of F_n, which precluded linearizing the Bernoulli Eqs., the non-linear solver produced nearly indistinguishable slip for $\zeta = 0.6$ and 0.96. At such large $I = N/2$, the best initial guess was to make all initial F_n coefficients equal to 0.01, rather than using results from the linearization, which were highly inaccurate.