A convergent boundary integral method for 3D interfacial flow with surface tension

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Drexel

Collaborators and References

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References:

D.M. Ambrose, M. Siegel, S. Tlupova. A small-scale decomposition for 3D boundary integral computations with surface tension. *Journal of Computational Physics*, **247**: 168-191, 2013.

D.M. Ambrose, Y. Liu, and M. Siegel. Convergence of a boundary integral method for 3D interfacial Darcy flow with surface tension. *Mathematics of Computation*, **86**:2745-2775, 2017.

Description of the Problems

- Two 3D fluids, one above the other, separated by a sharp interface.
- Horizontally, doubly periodic. Vertically, of infinite extent.
- Fluid velocities given by Darcy's Law: $\mathbf{V}_i = -K_i \nabla (p_i + \rho_i g z)$.
- Incompressible: $\nabla \cdot \mathbf{V}_i = 0$.
- $\mathbf{V}_1 \cdot \hat{\mathbf{n}} = \mathbf{V}_2 \cdot \hat{\mathbf{n}}$, but there is a jump in the tangential velocity.
- $p_1 - p_2 = \sigma \kappa$
- We let the free surface be given by $\mathbf{X}(\alpha, \beta, t)$. We write $\mathbf{X}_t = U\hat{\mathbf{n}} + V_1 \hat{\mathbf{t}}^{\mathbf{1}} + V_2 \hat{\mathbf{t}}^{\mathbf{2}}$.
- Putting this together, we have that $\mathbf{X}_t$ is like three derivatives of $\mathbf{X}$, so we can expect a third-order stiffness constraint from an explicit numerical method.

A Little History

- In 2D, Hou, Lowengrub, and Shelley (HLS) introduced a nonstiff method ('94, '97) for interfacial flow with surface tension.
- The HLS method for 2D problems was shown to converge (Ceniceros-Hou '98). Related convergence proofs by Beale-Hou-Lowengrub '96, Beale '01, Hou-Zhang '02.
- Using the HLS formulation, analysis was performed, showing well-posedness of the same initial value problems (A '03, '04, A-Masmoudi '05 and others).
- This was then generalized to analysis for the 3D initial value problems (A '07, A-Masmoudi '07, '09, and others such as Cordoba-Cordoba-Gancedo '13).
- Lessons learned from the analysis were then applied to devise a numerical method for the 3D problems (A-Siegel '12, A-Siegel-Tlupova '13).
- We have shown that a version of the 3D method converges (A-Liu-Siegel '17).

The Hou-Lowengrub-Shelley Method (2D)

- HLS introduced a non-stiff numerical method for 2D interfacial flow with surface tension.
- This involves making an arclength parameterization of the free surface, and computing using (θ, s_α) instead of Cartesian coordinates (x, y) :

$$\theta = \tan^{-1}\left(\frac{y_\alpha}{x_\alpha}\right), \qquad s_\alpha^2 = x_\alpha^2 + y_\alpha^2.$$

- The free surface has velocity $(x, y)_t = U\hat{\mathbf{n}} + V\hat{\mathbf{t}}$; from this, evolution equations for θ and s_α can be inferred.
- U is determined by physics, but V is chosen to maintain a favorable parameterization (e.g., arclength) from the equation $s_{\alpha t} = V_\alpha - \theta_\alpha U$.
- U is decomposed as its most singular part plus a remainder.
- With these choices, HLS are able to use a semi-implicit timestepping scheme and remove the stiffness constraint.

3D Numerical Method

- We replace the arclength parameterization with an isothermal parameterization:

$$E = \mathbf{X}_\alpha \cdot \mathbf{X}_\alpha = \mathbf{X}_\beta \cdot \mathbf{X}_\beta = G; \qquad F = \mathbf{X}_\alpha \cdot \mathbf{X}_\beta = 0.$$

- The tangential velocities, V_1 and V_2, are chosen to maintain the isothermal parameterization; an elliptic system, which can be solved spectrally, is satisfied by the tangential velocities.
- The Birkhoff-Rott integral must be computed; we use Ewald summation.
- We make a Small-Scale Decomposition of the evolution equations, separating out the most singular terms.
- We then use a semi-implicit timestepping method.

The Small-Scale Decomposition and Timestepping

- We write

$$\mathbf{X}^{n+1} - \Delta t \left(U_s^{n+1} \hat{\mathbf{n}}^n + V_{1s}^{n+1} \hat{\mathbf{t}}^{\mathbf{1}n} + V_{2s}^{n+1} \hat{\mathbf{t}}^{\mathbf{2}n} \right) = \mathbf{X}^n$$
$$+ \Delta t \left((U^n - U_s^n) \hat{\mathbf{n}}^n + (V_1^n - V_{1s}^n) \hat{\mathbf{t}}^{\mathbf{1}n} + (V_2^n - V_{2s}^n) \hat{\mathbf{t}}^{\mathbf{2}n} \right).$$

- Here, U_s^{n+1}, V_{1s}^{n+1}, and V_{2s}^{n+1} are the most singular parts of the velocities. For example:

$$U_s^{n+1} = -\frac{1}{2} \left(H_1 \left(\frac{\mu_\alpha^{n+1}}{\sqrt{E^n}} \right) + H_2 \left(\frac{\mu_\beta^{n+1}}{\sqrt{E^n}} \right) \right),$$

$$\mu^{n+1} = -B \left(\frac{\mathbf{X}_{\alpha\alpha}^{n+1} \cdot \hat{\mathbf{n}}^n + \mathbf{X}_{\beta\beta}^{n+1} \cdot \hat{\mathbf{n}}^n}{2E^n} \right) - W z^{n+1}.$$

- We have a linear system for $\mathbf{X}^{n+1}$, which we solve with preconditioned GMRES.

Results: Removing the Stiffness

- The above timestepping scheme is first-order in time; higher-order schemes are available, and we have also implemented a second-order version.
- Using our small-scale decomposition, we are able to effectively remove the stiffness from the problem.
- A fully explicit method would have a third-order stiffness constraint. We instead face only a first-order stiffness constraint.

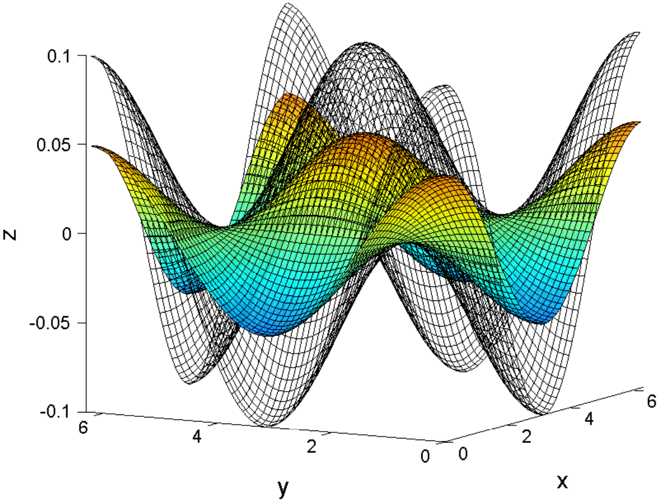
Table 3

Largest stable time step for the explicit and semi-implicit methods. The GMRES tolerance is 10^{-8}. Initial data is (62) with $A = 0.5$ for $W = 0$ and $A = 0.1$ for $W = 10$. The $W = 0$ runs are continued until the interface has nearly relaxed to a flat surface, and $W = 10$ runs are taken to $t = 0.4$.

N	Explicit			Implicit		
	$W = 0$, $B = 1.0$	$W = 0$, $B = 5.0$	$W = 10$, $B = 1.0$	$W = 0$, $B = 1.0$	$W = 0$, $B = 5.0$	$W = 10$, $B = 1.0$
32^2	5.0×10^{-4}	1.0×10^{-4}	5.0×10^{-4}	1.0×10^{-1}	2.0×10^{-2}	6.0×10^{-2}
64^2	6.25×10^{-5}	1.25×10^{-5}	6.25×10^{-5}	1.0×10^{-1}	2.0×10^{-2}	8.0×10^{-2}
128^2	7.8×10^{-6}	1.56×10^{-6}	7.8×10^{-6}	1.0×10^{-1}	2.0×10^{-2}	4.0×10^{-2}
256^2	1.0×10^{-6}	2.0×10^{-7}	1.0×10^{-6}	1.0×10^{-1}	2.0×10^{-2}	4.0×10^{-2}

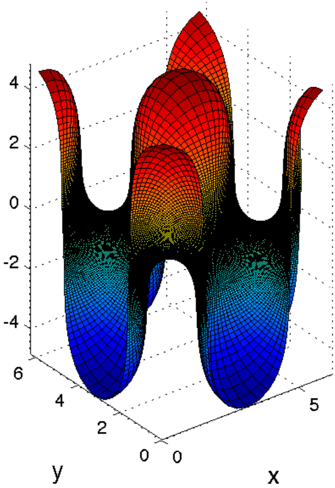
Results: A Relaxing Surface

- $A = 0.5$, $W = 0$, $N = 128^2$, $\Delta t = .0025$. Final time is $t = 1$.



Results: A Growing Finger

- $A = 0.1$, $W = 10$, $N = 256^2$, $\Delta t = 10^{-3}$ at first, and $\Delta t = 5 \times 10^{-4}$ later.



Convergence Analysis

- We want to prove convergence of (a version of) the numerical method.
- In 2D, there are convergence proofs of the HLS method (Ceniceros-Hou) and of a boundary integral method for water waves (Beale-Hou-Lowengrub).
- In 3D, there are convergence proofs for boundary integral methods for water waves (Beale; Hou-Zhang).
- We are unaware of such a proof of convergence for a 3D boundary integral method for interfacial flow with surface tension.
- To show convergence, we need to show consistency and stability.
- Consistency is fairly straightforward.

About Stability

- So, we want to prove stability for a version of our numerical scheme.
- This means that if we have a continuous surface $\mathbf{X}$, and a computed, discretized surface $\mathbf{X}_h$, we need to prove an estimate for the growth of $\mathbf{X} - \mathbf{X}_h$.
- We actually do this for the semi-discrete system (continuous in time, spatially discrete).
- The required estimates are very much like the energy estimates that we prove for continuous problems. However, for the continuous problem, the best quantity to estimate is κ, the mean curvature.

Summary So Far

- For computing, we can develop a small-scale decomposition for evolution of the free surface.
- Analytically, we get good estimates for curvature, but of course we need the surface as well; we went through a complicated procedure reconstructing a surface based on the curvature at each iteration.
- In the numerical analysis, we have a problem, then: we could make good estimates for curvature, but we are evolving the surface itself.
- Our goal is to find a version of the numerical method for which we can make the desired estimates; we would like the method to be as close as possible to what was implemented, but the main goal is to prove convergence of a boundary integral method for 3D interfacial flow with surface tension.

Important Ideas for Stability

- To prove stability, we prove energy estimates for the difference of the continuous solution, $\mathbf{X}$, and the computed solution, $\mathbf{X}_h$.
- These energy estimates are similar to the estimates of Ambrose and Ambrose-Masmoudi for related problems.
- Things are more difficult in the discrete setting since relationships may not hold exactly.
- Also, estimates work well for κ, but we need to evolve $\mathbf{X}$. Idea: decouple $\mathbf{X}$ and κ, before discretizing.
- With this key idea, plus the framework for estimates from Ambrose and Ambrose-Masmoudi, we are able to close the stability estimates.

Discretized System

- We have an evolution equation for $\mathbf{X}_h$:

$$\frac{d\mathbf{X}_h}{dt} = \mathcal{V}_h^0(\mathbf{X}_h, \kappa_h),$$

  with

$$\mathcal{V}_h^0 = \mathcal{U}_h \hat{\mathbf{n}}_h + \mathcal{V}_{1h}\mathbf{X}_{\alpha\mathbf{h}} + \mathcal{V}_{2h}\mathbf{X}_{\beta h},$$

  where the velocities are defined in terms of $\mathbf{X}_h$ and κ_h.

- We also have an evolution equation for κ_h :

$$\begin{aligned}\frac{d\kappa_h}{dt} =& -\frac{B}{4\sqrt{E_h}}\mathcal{L}_h^*\mathcal{L}_h\kappa_h + \frac{1}{2E_h}\left(R_h + \Delta_h T_h + \Delta_h K_h - \Delta_h C_n^h\right) \\ &+ \frac{\kappa_h}{2E_h}\left(2U_h L_h - 2D_{1h}V_{1h} + \frac{D_{1h}E_h}{E_h}V_{1h} - V_{2h}D_{2h}E_h\right) \\ &+ \frac{1}{2E_h}\left(D_{1h}\left(V_{1h}L_h + V_{2h}M_h\right) + D_{2h}\left(V_{1h}M_h + V_{2h}N_h\right)\right).\end{aligned}$$

About the Stability Estimate

- In the continuous case, if $\mathbf{X} \in H^0$ and $\kappa \in H^s$, then we can show $\mathbf{X} \in H^{s+2}$.
- In the discretized problem, we have broken the link between $\mathbf{X}_h$ and κ_h, and we can no longer draw this inference.
- This can be important, as the κ_h evolution equation will have $\mathbf{X}_h$ occuring, and we need certain regularity on $\mathbf{X}_h$ to complete the estimate.
- We have a solution to this: we replace $\mathbf{X}_h$ on the right-hand sides, where necessary, with

$$\Delta_h^{-1}(2\kappa_h \hat{\mathbf{n}}_h) + (\alpha_h, \beta_h, 0),$$

where

$$\hat{\mathbf{n}}_h = \mathbf{X}_{\alpha h} \times \mathbf{X}_{\beta h}.$$

- With this substitution, we still have consistency, and this allows the estimates to close.

The Main Theorem

We have the main theorem of A-Liu-Siegel '17:

Theorem

Suppose the problem is well-posed and has a sufficiently smooth solution $\mathbf{X}$ up to time $T > 0$. In addition we assume that $\mathbf{X}$ is nonsingular and satisfies certain bounds. Then the modified point vortex method is stable and 3^{rd}-order accurate. More precisely, there exists a positive number $h_0(T)$ such that for all $0 < h < h_0(T)$, we have

$$\|\mathbf{X} - \mathbf{X}_h\|_{L_h^2} \leq C(T)h^3, \tag{1}$$

where $\|\cdot\|_{L_h^2}$ is the discrete l^2 norm over a period of α, i.e., $\|\mathbf{x}\|_{L_h^2}^2 = \sum_{i,j=-N/2+1}^{N/2} |\mathbf{x}_{i,j}|^2 h^2$, and $C(T) > 0$ is a constant that does not depend on h.

Current and Future Work

- Allow for adaptive mesh refinement *via* overlapping coordinate patches.
- Parallelize the computation of the Birkhoff-Rott integral.
- Apply these tools to other physical problems (including computing, numerical analysis, and analysis); for example, hydroelastic waves.

Thanks for your attention.