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Convergence of the boundary integral method for interfacial stokes flow

Keyang Zhang
New Jersey Institute of Technology

ABSTRACT

CONVERGENCE OF THE BOUNDARY INTEGRAL METHOD FOR INTERFACIAL STOKES FLOW

by
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Boundary integral numerical methods are among the most accurate methods for interfacial Stokes flow, and are widely applied. They have the advantage that only the boundary of the domain must be discretized, which reduces the number of discretization points and allows the treatment of complicated interfaces. Despite their popularity, there is no analysis of the convergence of these methods for interfacial Stokes flow. In practice, the stability of discretizations of the boundary integral formulation can depend sensitively on details of the discretization and on the application of numerical filters. A convergence analysis of the boundary integral method for Stokes flow is presented focusing on a variant of the method of [22] for computing the evolution of an elastic capsule in two dimensional strain and shear flows. The analysis clarifies the role of numerical filters in practical computations.

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by
Keyang Zhang

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Department of Mathematical Sciences, NJIT
Department of Mathematics and Computer Science, Rutgers-Newark

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APPROVAL PAGE

CONVERGENCE OF THE BOUNDARY INTEGRAL METHOD FOR INTERFACIAL STOKES FLOW

Keyang Zhang

Dr. Michael S. Siegel, Dissertation Advisor — Date
Professor of Mathematical Sciences, NJIT

Dr. David M. Ambrose, Dissertation Co-Advisor — Date
Professor of Mathematical Sciences, Drexel University

Dr. Shidong Jiang, Committee Member — Date
Professor of Mathematical Sciences, NJIT

Dr. Yassine Boubendir, Committee Member — Date
Professor of Mathematical Sciences, NJIT

Dr. Brittany D. Hamfeldt, Committee Member — Date
Associate Professor of Mathematical Sciences, NJIT

BIOGRAPHICAL SKETCH

Author: Keyang Zhang

Degree: Doctor of Philosophy

Date: December 2020

Undergraduate and Graduate Education:

- Doctor of Philosophy in Mathematical Sciences,
  New Jersey Institute of Technology, Newark, NJ, 2020
- Master of Science in Mathematics,
  New York University, New York, NY, 2014
- Honor Bachelor of Science in Mathematics,
  University of Utah, Salt Lake City, UT, 2012

Major: Applied Mathematics

To my beloved parents...

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CHAPTER 1

INTRODUCTION

Boundary integral (BI) methods, or BIM, are among the most popular methods for computing interfacial fluid flow. They have been applied to compute the evolution of vortex sheets in the Kelvin-Helmholtz and Rayleigh-Taylor instabilities [5],[39],[43], Hele-Shaw flow [25],[31],[15], water waves [9],[26], and crystal growth [30],[42]. They have also been extensively applied in Stokes flow to simulate the evolution of drops, bubbles, elastic capsules and vesicles [44],[36],[22]. The methods only apply in problems that have a Green's function formulation. In fluid dynamics, this includes the important special cases of potential flow and Stokes flow. They also apply to boundary value problems outside of fluid dynamics, including linear elasticity, electrostatics, electromagnetic wave propagation (i.e., the Helmholtz equation) and related areas [14],[19].

The main advantage of boundary integral methods is that they reduce the dimension of the problem by involving only surface quantities [36], which both simplifies the handling of complex geometries and reduces the number of discretization points. Another significant advantage is that they can be made to have high accuracy. Boundary integral methods use a sharp interface formulation, and in contrast to so-called interface capturing methods such as the level-set or the immersed boundary method they do not lose accuracy due to 'smearing' of the interface. Spectrally accurate discretizations of boundary integral formulations have been implemented for 2D interfacial flow, see [27],[28],[35] and references therein. High order accurate discretizations of axisymmetric and 3D flow problems, although still a subject of current research, are increasingly common [41], [47]. As a result, boundary integral methods are a good choice in problems that demand high accuracy.

One of the greatest challenges in the practical implementation of boundary integral methods for time evolution problems is that they are very sensitive to numerical instabilities. If left uncontrolled, these instabilities will dominate and adversely affect the accuracy of computations. Numerical instabilities have been observed in surface and interfacial wave calculations for inviscid fluids by Longuet-Higgins and Cokelet [32], Baker, Meiron and Orszag [6], and Dold [17]. In these prior research, the instability was delayed but not completely eliminated by the application of smoothing techniques.

Computations of interfacial flows with surface or elastic membrane tension are much more sensitive to numerical instabilities due to the presence of high-order spatial derivatives. Straightforward discretizations of surface tension terms may lead to numerical instabilities. Pullin [39] experienced this difficulty first in computations of inviscid interfacial flow. Utilizing a boundary integral method for two fluid interfacial flows, Pullin noticed that small-scale corrugations appeared in regions of high curvature when surface tension is present. Eventually, the appearance of numerical instability linked with surface tension led to breakdown of the computations.

Linear analysis of discrete equations about equilibrium has identified common sources of numerical instabilities in BIM. For example, Baker and Nachbin [4] applied normal mode analysis to several BI schemes to study the linear evolution of periodic perturbations of a flat vortex sheet. With this linear analysis, they were able to identify common reasons for numerical instability. However, their research did account for the influence of nonlinearites and perturbations far from equilibrium.

Another major challenge in numerical simulations of interfacial flows with surface tension, especially with elastic membranes, is numerical stiffness associated with the time discretization. Here stiffness means that there is a constraint that the time-step size must depend on the spatial-step size. The stiffness is due to terms with high-order derivatives introduced into the interface dynamics by surface tension. This kind of numerical stiffness can be removed by utilizing implicit methods, but since the high derivatives are inside nonlocal operators, this is difficult to implement efficiently.

In [25], Hou, Lowengrub and Shelley, hereafter referred to as HLS, developed an efficient method to remove the high-order stiffness in computing the motion of fluid interfaces with surface tension in two-dimensional, irrotational and incompressible fluids. Their scheme is based on a boundary integral formulation using two natural variables: the tangent angle θ, and an equal-arclength parameter α, so that $\frac{\partial s}{\partial \alpha}$ is constant in α (here $s(\alpha, t)$ measures arclength from a reference point at $\alpha = 0$). This BI formulation is called the $\theta - s_\alpha$ formulation. We adapt this formulation to Stokes flow with elastic surfaces in our work. HLS further reformulate the equations to isolate the leading order stiff terms in such a way that they can then be treated implicitly in time discretizations in an efficient way [25], [24].

There are relatively few analyses of the convergence of BI methods. Beale, Hou and Lowengrub [9], hereafter referred to as BHL, gave a convergence proof of a BI method for water waves in two dimensions with or without surface tension. Applying a framework developed in [8] for linearized motion perturbed about an arbitrary smooth solution, BHL discovered that very delicate balances among terms in singular integrals and derivatives must be preserved at the discrete level in order to ensure numerical stability. They also noticed that numerical filtering is necessary at certain places to prevent the discretization from producing new instabilities in the high modes. This filtering depends on the particular approach for approximating spatial derivatives and quadrature rules for singular integrals. Ceniceros and Hou [13] generalized the analysis of [9] to include two-phase flow and surface tension, using the $\theta - s_\alpha$ formulation of [25]. Hou and Zhang [26] generalized the analysis of [9] to 3D. Ambrose, Liu and Siegel [3] prove convergence of a boundary integral method for 3D Darcy-law flow with surface tension.

Despite the significance of the above mentioned stability and convergence analysis for boundary integral methods in the water wave problem, there is no convergence analysis that we are aware of for the important case of interfacial Stokes flow. In this research, we provide such an analysis. The main difficulty of this analysis, compared to previous convergence studies for water waves, is a more complicated boundary integral formulation for the Stokes problem, and the presence of high derivatives in the boundary condition for an elastic membrane.

In the analyses of the stability of our method, we make significant use of the stabilizing effects of the highest derivative or leading order terms (so-called parabolic smoothing) to control lower order terms. In the water wave problem, it was found that strategically placed numerical filtering was necessary to prevent instabilities due to aliasing error from growing and destroying the computation. We similarly find that a targeted application of numerical filtering is necessary to prove stability in the Stokes-interface problem. This is consistent with numerical implementations of spectrally accurate methods for the evolution of drops, bubbles and elastic capsules in Stokes flow [22],[46],[35], which also find the need for some form of numerical filtering for stability. However, to make use of the parabolic smoothing, we find it important that numerical filtering *not* be applied to the leading order or highest derivative terms. Based on the analysis, we present a numerical scheme that utilizes a minimal amount of filtering yet is provably stable.

For concreteness, we consider the problem of the evolution of a Hookean elastic capsule in 2D Stokes flow, for an externally imposed straining or shearing flow. An elastic capsule is a drop or bubble that is enclosed by a thin, elastic membrane and suspended in an external liquid. It serves as a simple mechanical model of a cell or vesicle that is deformed by a fluid flow. Numerical studies of capsules in fluid flow have been performed with various membrane constitutive laws including Hookean [10], [22], neo-Hookean or Skalac [16], [45], and inextensible membranes [44]. Pozrikidis

[38] gives an overview of some of the early numerical studies of capsules in fluid flow, while a more recent review is provided by Barthes-Biesel [7].

In this research, we adapt a spectrally accurate numerical method for the evolution of a capsule in an extensional flow that was developed in [22]. The method of [22] was developed for the special case of an inviscid interior fluid and zero bending stress on the membrane surface. We generalize the method to include both a nonzero membrane bending stress and a viscous interior fluid, and analyze its convergence. For the closely related problem of: (i) an inviscid bubble or viscous drop, or (ii) an inextensible vesicle membrane evolving in an extensional Stokes flow, nonstiff BI methods have been by developed by Xu et al. [46], Veerapaneni et al. [44], and Sohn et al. [40] and extensively used in simulations. The nonstiff method for elastic capsules analyzed in this research is adapted from the method for drops in Xu et al. [46] to include Hookean membrane tension and interfacial bending stresses. We utilize the arclength-angle formulation of [25],[46],[27] to remove the numerical stiffness. Our reformulation makes use of a complex-variable description of the problem known as the Sherman−Lauricella formulation. Nonlocal convolution integrals in this formulation can be computed using spectrally accurate alternate point trapezoidal rule [23].

The governing equations for our problem are presented in Chapter 2. The BI formulation is presented in Chapter 3. For our BI formulation, we present in Chapter 4 a spectrally accurate numerical discretization. Several preliminary lemmas are stated and proven in Chapter 5 which provide error estimates on numerical differentiation, integration, and filtering operators. We then prove consistency of our numerical method in Chapter 6. The statement of the main convergence theorem, Theorem 7.0.2, is given in Chapter 7. Some preliminary estimates used in the proof of stability are given Chapters 8 and 9. Evolution equations for the errors are presented in Chapter 10, and energy estimates and the final proof of stability and Theorem 7.0.2

are given in Chapter 11. Concluding remarks are provided in Chapter 12. A proof of a critical lemma and estimates of nonlinear terms in the variation are given in the Appendix.

CHAPTER 2

PROBLEM FORMULATION

We present the governing equations for a single elastic capsule in 2D Stokes flow. The exterior fluid domain is denoted by Ω, and we use a superscript i for variables and parameters in the inner fluid, and the membrane surface is given by $\partial\Omega = \gamma$.

The drop and exterior fluid are assumed to have the same density, so gravitational effects are absent. On γ the unit normal vector $\mathbf{n}$ points toward the exterior fluid. The unit tangent $\mathbf{t}$ points in the direction such that the interior fluid is to the right as γ is traversed clockwise. We define an angle θ measured counterclockwise positive from the positive $x-$axis to $\mathbf{t}$. The geometry is illustrated in Figure 2.1. The local curvature of the interface is $\kappa = -\frac{\partial\theta}{\partial s}$ and is positive when

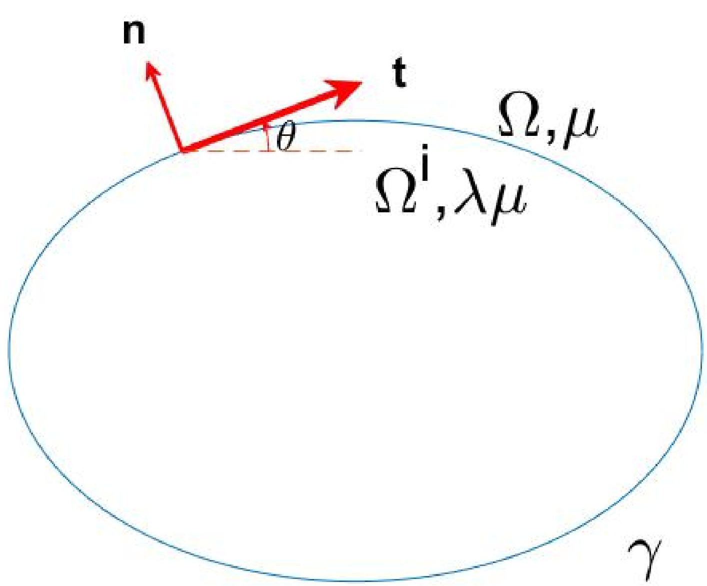

Figure 2.1 Fluid drop with viscosity $\lambda\mu$ occupying region Ω^i is immersed in a fluid with viscosity μ occupying region Ω

the shape is convex. Here, s is an arclength parameter that increases as γ is traversed clockwise.

In dimensionless form, the Stokes equations governing fluid flow are:

$$\begin{cases} \Delta \mathbf{u} = \nabla p,\ \nabla \cdot \mathbf{u} = 0, \quad \mathbf{x} \in \Omega, & (2.1) \\ \lambda \Delta \mathbf{u}^i = \nabla p^i,\ \nabla \cdot \mathbf{u}^i = 0, \quad \mathbf{x} \in \Omega^i, & (2.2) \end{cases}$$

where $p(\mathbf{x})$ and $\mathbf{u}(\mathbf{x})$ are the pressure and velocity fields and $\lambda = \frac{\mu^i}{\mu}$ is the viscosity ratio. The fluid velocity is taken to be continuous across the interface, i.e., $\mathbf{u}(\mathbf{x}) = \mathbf{u}^i(\mathbf{x})$ for $\mathbf{x} \in \gamma$.

The area enclosed by the capsule is conserved, and lengths are nondimensionalized by the radius R of the circular capsule with the same area. Velocities are nondimensionalized by U, where U will be specified below. Time is nondimensionalized by $\frac{R}{U}$, and pressure by $\frac{U\mu}{R}$. At $t = 0$ the capsule can have arbitrary shape and membrane tension.

The no slip condition on the capsule surface is given by

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, t) \quad \text{for } \mathbf{x} \in \gamma, \tag{2.3}$$

Equation (2.3) satisfies the kinematic condition that $\frac{d\mathbf{x}}{dt} \cdot \mathbf{n} = \mathbf{u} \cdot \mathbf{n}$ on γ. The far-field boundary condition is taken to be a general incompressible linear flow:

$$\lim_{|\mathbf{x}| \to \infty} \mathbf{u}(\mathbf{x}) = \mathbf{u}_\infty(\mathbf{x}) = \begin{pmatrix} Q & B + \frac{G}{2} \\ B - \frac{G}{2} & -Q \end{pmatrix} \mathbf{x}, \tag{2.4}$$

where the dimensionless parameter (Q, B, G) are equal to their dimensional counterparts Q_∞, etc, times the time scale $\frac{R}{U}$; i.e., $(Q, B, G) = \frac{R}{U}(Q_\infty, B_\infty, G_\infty)$. The far-field flow is a pure strain if $B = G = 0$, and a linear shear flow if $Q = 0$ and $G = 2B$. At the elastic membrane interface, we have the additional boundary condition that the total interfacial stress $\mathbf{f}$ is balanced by the jump in fluid stress across the interface:

$$\left[T \cdot \mathbf{n}\right] = \mathbf{f}, \tag{2.5}$$

where $T = -p + 2E_{ij}$ and $T^i = -p^i + 2\lambda E^i_{ij}$, and where:

$$E_{ij} = \frac{1}{2}\Big(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\Big), \tag{2.6}$$

is the stress tensor. Here $\big[\,\cdot\,\big]$ denotes the jump:

$$\big[\mathbf{g}\big] = \mathbf{g} - \mathbf{g}^i \quad \text{for } \mathbf{x} \in \gamma. \tag{2.7}$$

An expression for the interfacial stress $\mathbf{f}$ on the right hand side of Equation (2.5) is obtained in [37] by an analysis of interfacial forces and torques, or more specifically, interfacial tensions and bending moments. The result is given in Equation (3.16) of [37], which in our notation is:

$$\mathbf{f} = -\frac{\partial}{\partial s}\big(\mathcal{S}\mathbf{t} + q_B\mathbf{n}\big) \tag{2.8}$$

where $\mathcal{S} = \mathcal{S}(s)$ is the surface tension, and $q_B(s) = \frac{dm_B}{ds}$ with $m_B = m_B(s)$ the bending moment. The constitutive equation for the bending moment m is assumed to be the simple linear relation:

$$m_B(s) = \kappa_B\kappa(s) \tag{2.9}$$

where κ_B is the (dimensionless) bending modulus, and $\kappa(s)$ is the interfacial curvature. For the sake of simplicity, we consider a membrane with a Hookean or linear elastic response, for which the dimensional tension is given by [36]:

$$\tilde{\mathcal{S}} = E(\eta - 1),\, \eta = \frac{\partial s}{\partial s_R}. \tag{2.10}$$

Here η is the stretch ratio between arclength s of the membrane at time t, and arclength s_R in a reference configuration in which there is no tension in the membrane. The tension is nondimensionalized by E, so that in dimensionless form:

$$\mathcal{S} = \eta - 1. \tag{2.11}$$

We also now define the characteristic velocity which is used for nondimensionalization as $U = \frac{E}{\mu}$.

CHAPTER 3

BOUNDARY INTEGRAL FORMULATION

A boundary integral formulation for an elastic capsule or vesicle in 2D Stokes flow with an inextensible membrane is given by Veerapaneni et al. [44]. Their formulation uses a single layer potential $S[\mathbf{f}](\mathbf{x})$ to represent the velocity, where:

$$S[\mathbf{f}] = \int_\gamma G_s(\mathbf{x}, \mathbf{y})\mathbf{f}(\mathbf{y})ds_{\mathbf{y}}, \tag{3.1}$$

and where the 2D Stokes free space kernel G_s is given by:

$$G_s(\mathbf{x}, \mathbf{y}) = \frac{1}{4\pi}\Big(- \ln \rho \mathbf{I} + \frac{\mathbf{r} \otimes \mathbf{r}}{\rho^2}\Big), \quad \mathbf{r} = \mathbf{x} - \mathbf{y}, \quad \rho = \|\mathbf{r}\|_2. \tag{3.2}$$

Because of the log singularity in G_s, Veerapaneni et al. [44] employ a special form of Gauss−Legendre quadrature due to Alpert [2] to discretize the integral. While accurate, this quadrature is rather complicated and for this and other reasons an analysis of the discrete equations for their method is difficult. We instead adapt the Sherman-Lauricella formulation [29],[27] to the membrane problem. This is a complex variable formulation, for which the primitive variables are expressed in terms of integral over a single complex density that is defined on the drop interface and satisfies a Fredholm second kind equation. It has been used to solve Stokes equations for fluid flow in [29],[46],[20],[27],[28]. This formulation will be more convenient for analysis.

A stream function is introduced for each region, so that:

$$(u_1, u_2) = (W_{x_2}, -W_{x_1}), \quad \mathbf{x} \in \Omega,$$
$$(u_1^i, u_2^i) = (W_{x_2}^i, -W_{x_1}^i), \quad \mathbf{x} \in \Omega^i. \tag{3.3}$$

The formulation for each region is similar, so we focus on the exterior region.

The curl of Equations (2.1)−(2.2) implies that:

$$\nabla^4 W = 0, \quad \mathbf{x} \in \Omega, \tag{3.4}$$

i.e., $W(x_1, x_2) = u_1(x_1, x_2) + iu_2(x_1, x_2)$ is a biharmonic function, and similarly for $W^i(x_1, x_2) = u_1^i(x_1, x_2) + iu_2^i(x_1, x_2)$. It follows that $W(x_1, x_2)$ has a Goursat representation:

$$W(x_1, x_2) = \mathrm{Re}\big(\overline{z} f(z) + h(z)\big), \quad z \in \Omega, \tag{3.5}$$

where $f(z)$ and $g(z)$ are analytic functions of the complex variable $z = x_1 + ix_2$ on Ω ([15],[11]).

The functions $f(z)$ and $g(z) = h'(z)$ are known as Goursat functions. Similarly, $W^i(x_1, x_2) = \mathrm{Re}\big(\overline{z} f^i(z) + h^i(z)\big)$ for $z \in \Omega^i$, where $f^i(z)$ and $h^i(z)$, with $g^i(z) = h^{i'}(z)$, are analytic in Ω^i.

The primitive variables and their spatial derivatives in the exterior and interior regions can be expressed in terms of the Goursat functions; see, for example, [30]. In the exterior domain, $z \in \Omega$,

$$-u_2 + iu_1 = f(z) + z\overline{f'(z)} + \overline{g(z)}, \tag{3.6}$$

$$q + ip = -4f'(z), \tag{3.7}$$

$$E_{11} + iE_{12} = -E_{22} + iE_{21} = -i\big(z\overline{f''(z)} + \overline{g'(z)}\big). \tag{3.8}$$

Here, q is the fluid vorticity, with $\boldsymbol{\omega} = \nabla \times \boldsymbol{u} = \big(\partial_{x_1} u_2 - \partial_{x_2} u_1\big)\boldsymbol{e}_3 = q\boldsymbol{e}_3$. Analogous expressions hold for the interior domain, with the exception that $q^i + i\left(\frac{p^i}{\lambda}\right) = 4f^{i'}(z)$ for $z \in \Omega^i$.

As shown in [11], the far-field velocity conditions imply that:

$$f(z) = \frac{G}{4}z + H(t) + O(|z|^{-2}),$$
$$g(z) = -(B + iQ)z + \overline{H(t)} + O(|z|^{-2}), \tag{3.9}$$

as $|z| \to \infty$, where $H(t)$ is an as yet arbitrary function of time.

The surface stress exerted on the interface γ by material in the exterior domain, per Equation (2.5), is $-p\mathbf{n} + 2\mathbf{E} \cdot \mathbf{n} = (f_1, f_2)$, which has complex counterpart:

$$f_1 + i f_2 = 2\frac{\partial}{\partial s}\Big\{ \lim_{z \to \tau^+} \big(f(z) - z\overline{f'(z)} - \overline{g(z)} \big) \Big\}, \tag{3.10}$$

where the limit indicates that z approaches a point τ on γ from the exterior domain. A similar expression multiplied by λ holds for the surface stress due to material in the interior domain. The difference is equal to the total interfacial stress $\mathbf{f}$ given in Equation (2.8). The stress balance condition can be integrated with respect to s to obtain:

$$\begin{aligned} \lim_{z \to \tau^+} \big(f(z) - z\overline{f'(z)} - \overline{g(z)} \big) - \lambda \lim_{z \to \tau^-} \big(f^i(z) - z\overline{f^{i\prime}(z)} - \overline{g^i(z)} \big) \\ = -\frac{1}{2}\big((\mathcal{S} + \kappa_B \kappa^2)\tau_s - \kappa_B \tau_{sss} \big), \end{aligned} \tag{3.11}$$

where $\mathcal{S} = \mathcal{S}(\tau, t)$. The right hand side of (3.11) is the complex counterpart of Equations (2.8), (2.9). The freedom of choice in specifying the Goursat functions allows us to set to zero a function of time that results from the integration.

In the Sherman-Lauricella formulation, the Goursat functions are written in terms of Cauchy-type integrals that contain a single complex density $\omega(z, t)$, defined on the time-evolving interface γ, and where the integrals give the modification to the imposed far-field flow that is caused by the drop. The representation is such that, if we introduce:

$$\begin{aligned} f^o(z) &= \frac{1}{2\pi i}\int_\gamma \frac{\omega(\zeta, t)}{\zeta - z} d\zeta + \frac{Gz}{4} + H(t), \\ g^o(z) &= \frac{1}{2\pi i}\int_\gamma \frac{-\overline{w(\zeta, t)}d\zeta + w(\zeta, t)d\bar{\zeta}}{\zeta - z} - \frac{1}{2\pi i}\int_\gamma \frac{\bar{\zeta}\omega(\zeta, t)}{(\zeta - z)^2} d\zeta \\ &\quad - (B + iQ)z - \overline{H(t)}, \end{aligned} \tag{3.12}$$

then the Goursat functions are given by:

$$\begin{aligned}(f(z),g(z)) &= (f^o(z),g^o(z)), \quad \text{when } z\in\Omega,\\ (f^i(z),g^i(z)) &= (f^o(z),g^o(z)), \quad \text{when } z\in\Omega^i. \end{aligned} \tag{3.13}$$

Here, z is an arbitrary point in the complex plane away from the interface γ, and ζ is the variable of integration on the interface contour. In the definitions (Equation (3.12)), $\int_\gamma$ can denote integration around γ in either the counterclockwise direction, as is the usual convention in the complex plane, or clockwise; the difference is resolved by a change in sign of $\omega(\zeta,t)$, and we choose the clockwise direction.

From the definitions (Equation (3.12)), the Goursat functions are analytic functions of z except for z on the contour γ. They are also singular as $z\to\infty$ to accommodate the imposed flow. The Sherman−Lauricella integral equation is constructed when the representation of the Goursat functions in terms of ω of Equation (3.12) to (3.13) is substituted into the stress-balance boundary condition (Equation (3.11)). As z approaches a point τ on γ, some of the Cauchy-type integrals that result have local, simple pole contributions from a neighborhood of $z=\tau$ that can be evaluated by the Plemelj formula [15], and the remaining part of these integrals is of principal value type. The final form that the equation takes can be written as:

$$\begin{aligned}\omega(\tau,t)+&\frac{\beta}{2\pi i}\int_\gamma \omega(\zeta,t)d\ln\left(\frac{\zeta-\tau}{\overline{\zeta}-\overline{\tau}}\right)+\frac{\beta}{2\pi i}\int_\gamma \overline{\omega(\zeta,t)}d\frac{\zeta-\tau}{\overline{\zeta}-\overline{\tau}}\\ &+\beta(B-iQ)\overline{\tau}+2\beta H(t) = -\frac{\chi}{2}\big((\mathcal{S}+\kappa_B\kappa^2)\tau_s-\kappa_B\tau_{sss}\big),\end{aligned} \tag{3.14}$$

where $\beta=\frac{1-\lambda}{1+\lambda}$ and $\chi=\frac{1}{1+\lambda}$. The apparent singularity at $\zeta=\tau$ in the two integrals on the left−hand side is removable. The choice that:

$$H(t)=\frac{1}{2}\int_\gamma \omega(\zeta,t)ds \tag{3.15}$$

removes a rank deficiency of the integral equation (3.14) in the limit when $\lambda = 0$ of an inviscid drop (see, for example, [4] and [11]), and $H(t) \equiv 0$ as a consequence of the constant area of the interior region Ω^i.

The fluid velocity on the interface is found from Equation (3.6) by letting z approach a point τ on γ from either Ω or Ω^i. The representation of the Goursat functions in terms of $\omega(z,t)$ of Equation (3.12) to Equation (3.13) is such that the local, simple pole contributions to Equation (3.6) from the integrals near $z = \tau$ cancel as $z \to \tau^{\pm}$. The fluid velocity is therefore continuous automatically across the interface and is given by:

$$(u_1 + iu_2)|_\gamma = -\frac{1}{2\pi}\text{P.V.}\int_\gamma \omega(\zeta,t)\Big(\frac{d\zeta}{\zeta-\tau} + \frac{d\overline{\zeta}}{\overline{\zeta}-\overline{\tau}}\Big) + \frac{1}{2\pi}\int_\gamma \overline{\omega(\zeta,t)}\, d\frac{\zeta-\tau}{\overline{\zeta}-\overline{\tau}} + (Q+iB)\overline{\tau} - \frac{iG}{2}\tau \tag{3.16}$$

on the interface γ. The apparent singularity for ζ near τ in the second integral is removable, but in the first integral the P.V. indicates that it is to be interpreted as a Cauchy principal value integral.

The fluid velocity on the interface, in terms of its normal and tangential components u_n and u_s, is $\boldsymbol{u} = u_n\boldsymbol{n} + u_s\boldsymbol{t}$, where the complex counterparts of the unit vectors $\boldsymbol{n}$ and $\boldsymbol{t}$ are n and s_T with $s_T = -in = \partial_s\tau$. It follows that:

$$u_n = \text{Re}\big\{(u_1+iu_2)|_\gamma\overline{n}\big\} \quad \text{and} \quad u_s = -\text{Im}\big\{(u_1+iu_2)|_\gamma\overline{n}\big\}, \tag{3.17}$$

on the interface γ.

For the numerical discretization of Equation (3.14), we introduce an equal arclength parametrization of the interface γ. This is constructed following Hou, Lowengrub and Shelley [25], and is an essential component of the method for removing the stiffness.

The spatial parametrization of the interface is given by $\alpha \in [0, 2\pi)$, and a point τ on the interface has Cartesian coordinates (x_1, x_2), so that $\tau = x_1(\alpha,t) + ix_2(\alpha,t)$.

The unit tangent vector s_T and normal n in complex form are $s_T = \frac{\partial \tau}{\partial s} = \frac{\tau_\alpha}{s_\alpha} = \exp(i\theta)$ and $n = is_T = i\exp(i\theta)$. Differentiation with respect to time implies that

$$\tau_{\alpha t} = s_{\alpha t} e^{i\theta} + s_\alpha \theta_t i e^{i\theta}. \tag{3.18}$$

When $\tau = \tau_m$ is a material point on the interface its velocity is equal to the local fluid velocity, per Equation (2.5), so that:

$$\frac{d\tau_m}{dt} = u_n i e^{i\theta} + u_s e^{i\theta}, \tag{3.19}$$

where the subscript m is used to denote material point.

However, the shape of the evolving interface is determined by the normal velocity component u_n alone. Although u_s has physical meaning as the tangential component of the fluid velocity, if u_s is replaced by any other smooth function $\phi_s(\alpha, t)$ in (3.19), then τ still lies on the interface but is no longer a material point, and the role of ϕ_s is simply to implement a specific choice of $\tau \in \gamma$ and the interface parametrization via α, without changing the interface shape or evolution. The interfacial velocity generated by using ϕ_s instead of u_s is denoted in the complex form by:

$$v = \frac{d\tau}{dt} = u_n i e^{i\theta} + \phi_s e^{i\theta}. \tag{3.20}$$

When this is done, differentiation of (3.20) with respect to α gives a second relation for $\tau_{\alpha t}$,

$$\tau_{\alpha t} = \big((\phi_s)_\alpha - u_n\theta_\alpha\big)e^{i\theta} + \big((u_n)_\alpha + \phi_s\theta_\alpha\big)ie^{i\theta}. \tag{3.21}$$

Equating (3.18) and (3.21), we have:

$$s_{\alpha t} = (\phi_s)_\alpha - u_n\theta_\alpha, \tag{3.22}$$

$$\theta_t = \frac{1}{s_\alpha}\big((u_n)_\alpha - \phi_s\theta_\alpha\big), \tag{3.23}$$

where γ is now described parametrically by $s = s(\alpha, t)$ and $\theta = \theta(\alpha, t)$ instead of $x_1 = x_1(\alpha, t)$ and $x_2 = x_2(\alpha, t)$.

The equal arclength frame is chosen by setting $s_\alpha = s_\alpha(t)$ to be spatially constant along the interface, so that it varies in time only. Then since s_α is always equal to its mean around γ, it follows from Equation (3.22) that:

$$s_{\alpha t} = (\phi_s)_\alpha - u_n\theta_\alpha = -\frac{1}{2\pi}\int_0^{2\pi} u_n\theta_{\alpha'}d\alpha'. \tag{3.24}$$

Integration of the second of these equations with respect to α implies that:

$$\phi_s(\alpha, t) = \partial_\alpha^{-1}\big(u_n\theta_\alpha - \langle u_n\theta_\alpha\rangle\big), \tag{3.25}$$

where

$$\langle f\rangle = \frac{1}{2\pi}\int_0^{2\pi} f(\alpha')d\alpha' \tag{3.26}$$

is the mean of f, and ∂_α^{-1} is defined for a function f with zero mean as

$$\partial_\alpha^{-1} f = \sum_{\substack{k=-\infty \\ k\neq 0}}^{\infty} \frac{\hat{f}_k}{ik}e^{ik\alpha}. \tag{3.27}$$

In the above, $\hat{f}_k$ are the Fourier coefficients of f. Also, an arbitrary function of time has been set so that $\phi_s(\alpha, t)$ has zero mean. This gives the required tangential velocity ϕ_s of the equal arc length frame.

When (3.25) is substituted into Equations (3.22) and (3.23), the system by which the dynamics of the interface is tracked becomes:

$$s_{\alpha t} = -\frac{1}{2\pi}\int_0^{2\pi} u_n\theta_{\alpha'}d\alpha', \tag{3.28}$$

$$\theta_t = \frac{1}{\sigma}\Big[\theta_\alpha\partial_\alpha^{-1}\big(u_n\theta_\alpha - \langle u_n\theta_\alpha\rangle\big) + (u_n)_\alpha\Big]. \tag{3.29}$$

At each time step (3.28) and (3.29) are integrated forward in time, and (s_α, θ) are mapped to the Cartesian coordinates (x_1, x_2) of points on γ. The map is given by integration of $\tau_\alpha = s_\alpha e^{i\theta}$ with respect to α and is:

$$x_1(\alpha,t) = x_{1c}(t) + s_\alpha(t)\partial_\alpha^{-1}(\cos(\theta(\alpha',t))), \tag{3.30}$$

$$x_2(\alpha,t) = x_{2c}(t) + s_\alpha(t)\partial_\alpha^{-1}(\sin(\theta(\alpha',t))), \tag{3.31}$$

where $(x_{1c}(t), x_{2c}(t))$ is the constant Fourier mode of $(x_1(\alpha,t), x_2(\alpha,t))$, which is evolved from Equation (3.20) as:

$$\frac{d}{dt}(x_{1c}(t) + ix_{2c}(t)) = \hat{v}_0(t) = \langle v \rangle, \tag{3.32}$$

where $\hat{v}_0(t)$ is the $k = 0$ Fourier mode of interface velocity v.

Membrane tension:

A formula for the membrane tension $\mathcal{S}(\alpha,t)$ in terms of interface shape $\tau(\alpha,t)$ and the initial tension $\mathcal{S}(\alpha,0)$ is required to close the system of Equations (3.14)-(3.17), (3.25), (3.28)-(3.32). We derive this formula by adapting the presentation in [22].

Recall that $\tau(\alpha,t)$ is a general nonmaterial parameterization of the interface at time t. Introduce a parameterization $\tau(\alpha_p,0)$ of the initial profile in terms of a Lagrangian or material coordinate α_p, and denote the location of the same material point at time $t > 0$ by $\tau(\alpha_m(\alpha_p,t),t)$; this serves as a definition of a 'forward' map $\alpha_m(\alpha_p,t)$. We also define the 'backward' map $\alpha_0(\alpha,t)$ such that $\tau(\alpha_0(\alpha,t),0)$ is the location at $t = 0$ of the material point that at time t is located at $\tau(\alpha,t)$. It follows that α_m and α_0 are one to one and inverses.

We desire a formula for $\mathcal{S}(\alpha,t)$ that gives the tension in terms of the initial state of the membrane. Write s_0 for arclength at time $t = 0$ and note from Equation (2.11) that for a Hooke's law membrane,

$$\mathcal{S}(s_0,0) = \frac{\partial s_0}{\partial s_R} - 1. \tag{3.33}$$

Then for $t > 0$,

$$\mathcal{S}(s,t) = \frac{\partial s}{\partial s_0}\frac{\partial s_0}{\partial s_R} - 1 = \frac{\partial s}{\partial s_0}\big(1 + \mathcal{S}(s_0, 0)\big) - 1. \tag{3.34}$$

We determine an equation for the time evolution of $\frac{\partial s}{\partial s_0}$. The arclength at time t is:

$$s(\alpha,t) = \int_0^{\alpha} s_\alpha(\alpha', t)d\alpha', \tag{3.35}$$

and the length of the same material arc at $t = 0$ is:

$$s_0(\alpha,t) = \int_{\alpha_0(0,t)}^{\alpha_0(\alpha,t)} s_\alpha(\alpha', 0)d\alpha'. \tag{3.36}$$

Hence, in terms of α,

$$\frac{\partial s}{\partial s_0} = \frac{s_\alpha(\alpha,t)}{s_\alpha(\alpha_0(\alpha,t),0)\alpha_0'(\alpha,t)}, \tag{3.37}$$

where $\alpha_0'(\alpha,t) = \frac{\partial \alpha_0}{\partial \alpha}(\alpha,t)$, so (3.34) becomes

$$\mathcal{S}(\alpha,t) = \frac{s_\alpha(t)}{s_\alpha(\alpha_0(\alpha,t),0)\alpha_0'(\alpha,t)}\big(1 + \mathcal{S}(\alpha_0(\alpha,0),0)\big) - 1, \tag{3.38}$$

where we have made use of the fact that $s_\alpha(\alpha,t) = s_\alpha(t)$ is spatially independent.

The formula for the membrane tension therefore requires an equation for the backward map $\alpha_0(\alpha,t)$. First, note that, by definition of α_m and α_p, the condition for the motion of a material particle becomes:

$$\frac{d}{dt}\tau(\alpha_m(\alpha_p,t),t) = u_1 + iu_2, \tag{3.39}$$

that is,

$$\left.\frac{\partial \tau}{\partial t}\right|_{\alpha} + \left.\frac{\partial \tau}{\partial \alpha}\frac{\partial \alpha_m}{\partial t}\right|_{\alpha_p} = u_1 + iu_2, \tag{3.40}$$

at $\alpha = \alpha_m(\alpha_p, t)$. An expression for $\left.\frac{\partial \tau}{\partial t}\right|_{\alpha}$ is given by Equation (3.20), i.e., which describes the motion of $\tau(\alpha,t)$ at a fixed α with normal velocity u_n and tangential velocity ϕ_s. Substitution of Equation (3.20) into Equation (3.40) yields the evolution equation for the forward map $\alpha_m(\alpha_p, t)$:

$$\left.\frac{\partial \alpha_m}{\partial t}\right|_{\alpha_p} = \frac{1}{\tau_\alpha}\big[u_1 + iu_2 - (u_n ie^{i\theta} + \phi_s e^{i\theta})\big] \tag{3.41}$$

at $\alpha = \alpha_m(\alpha_p, t)$.

The evolution of the backward map $\alpha_0(\alpha, t)$ is obtained by noting that α_m and α_0 are inverses, so that differentiation of the identity $\alpha = \alpha_m(\alpha_0(\alpha, t), t)$ with respect to time keeping α fixed implies

$$\left.\frac{\partial \alpha_m}{\partial t}\right|_{\alpha_p} + \frac{\partial \alpha_p}{\partial \alpha_m}\left.\frac{\partial \alpha_0}{\partial t}\right|_{\alpha} = 0, \tag{3.42}$$

where we have set $\alpha_p = \alpha_0(\alpha, t)$ in the first two derivatives. Differentiation of the same identity with respect to α keeping t fixed gives:

$$\frac{\partial \alpha_m}{\partial \alpha_p} = \left(\frac{\partial \alpha_0}{\partial \alpha}\right)^{-1}. \tag{3.43}$$

Eliminating α_m in favor of α_0 in (3.41), (3.42) and (3.43) gives the initial value problem for the backward map:

$$\begin{aligned} \left.\frac{\partial \alpha_0}{\partial t}\right|_{\alpha} &= \frac{\partial \alpha_0}{\partial \alpha}\frac{1}{\tau_\alpha}\big[u_n ie^{i\theta} + \phi_s e^{i\theta} - (u_1 + iu_2)\big] \\ &= \frac{\partial \alpha_0}{\partial \alpha}\frac{1}{\tau_\alpha}\big[(\phi_s - u_s)e^{i\theta}\big], \end{aligned} \tag{3.44}$$

which together with Equation (3.38) is the main result of this subsection.

In summary, the main equations that govern capsule evolution are given by Equations (3.14)-(3.17), (3.25), (3.28)-(3.32), (3.38), (3.44). A nonstiff numerical method for solving this system of equations is presented in the next chapter.

CHAPTER 4

NUMERICAL METHOD

We construct a continuous in time, discrete in space numerical scheme for the interfacial evolution equations by providing rules to approximate the spatial derivatives and singular integrals.

We discretize the spatial variable α by $\alpha_j = jh$, where $j = -\frac{N}{2}+1, \cdots, \frac{N}{2}$, so that α is defined on a uniform grid of mesh size $h = \frac{2\pi}{N}$. We define a discrete Fourier transform of a periodic function f whose values are known at $\alpha_j = jh$ by:

$$\hat{f}_k = \frac{1}{N} \sum_{j=-\frac{N}{2}+1}^{\frac{N}{2}} f(\alpha_j) e^{-ik\alpha_j}, \text{ for } k = -\frac{N}{2}+1, \cdots, \frac{N}{2}, \tag{4.1}$$

with the inverse transform given by:

$$f(\alpha_j) = \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} \hat{f}_k e^{ik\alpha_j}, \text{ for } j = -\frac{N}{2}+1, \cdots, \frac{N}{2}. \tag{4.2}$$

We compute spatial derivatives of f with a pseudo-spectral approximation, which we denote by $S_h f$. S_h is defined by:

$$\widehat{(S_h f)}_k = ik\hat{f}_k, \text{ for } k = -\frac{N}{2}+1, \cdots, \frac{N}{2}. \tag{4.3}$$

We denote by $\theta(\alpha_j)$, $\omega(\alpha_j)$, $\zeta(\alpha_j)$ etc. the exact continuous solution evaluated at grid points α_j, and by θ_j, ω_j, ζ_j etc the discrete approximation. Also, we use $\sigma(t)$ to denote the numerical approximation of $s_\alpha(t)$.

Sometimes we may need to apply numerical or spectral filtering to our discrete solution. Indeed, this will be critical for the stability of our method. Our numerical filtering is defined in Fourier space as follows [9]:

$$\widehat{(f^p)}_k = \rho(kh)\hat{f}_k, \tag{4.4}$$

where ρ is a cutoff function with the following properties:

$$\rho(-x) = \rho(x) \; ; \; \rho(x) \geq 0, \tag{i}$$

$$\rho(x) \in C^r \; ; \; r > 2, \tag{ii}$$

$$\rho(\pm\pi) = \rho'(\pm\pi) = 0, \tag{iii}$$

$$\rho(x) = 1 \text{ for } |x| \leq \mu\pi, \; 0 < \mu < 1. \tag{iv}$$

Condition (iv) ensures the spectral accuracy of the filtering. We define a filtered derivative operator D_h by

$$(\widehat{D_h f})_k = ik\rho(kh)\hat{f}_k, \text{ for } k = -\frac{N}{2} + 1, \cdots, \frac{N}{2}. \tag{4.5}$$

Before discretizing Equation (3.14), we first parametrize the integrals by α and rewrite the equation in the equivalent form (supressing time dependence):

$$\begin{aligned}
\omega(\alpha) + \frac{\beta}{2\pi i}\int_{-\pi}^{\pi} \Big\{ \omega(\alpha')\Big(& \frac{\zeta_\alpha(\alpha')}{\zeta(\alpha') - \tau(\alpha)} - \frac{\overline{\zeta_\alpha(\alpha')}}{\overline{\zeta(\alpha')} - \overline{\tau(\alpha)}}\Big) \\
& + \overline{\omega(\alpha')}\Big(\frac{\zeta_\alpha(\alpha')}{\overline{\zeta(\alpha')} - \overline{\tau(\alpha)}} - \frac{(\zeta(\alpha') - \tau(\alpha))}{(\overline{\zeta(\alpha')} - \overline{\tau(\alpha)})^2}\overline{\zeta_\alpha(\alpha')}\Big)\Big\} d\alpha' \\
& + \beta(B - iQ)\overline{\tau(\alpha)} + 2\beta H(t) = -\frac{\chi}{2}\Big(\mathcal{S}(\alpha)e^{i\theta(\alpha)} - \frac{\kappa_B \theta_{\alpha\alpha}(\alpha)}{s_\alpha^2} i e^{i\theta(\alpha)}\Big).
\end{aligned} \tag{4.6}$$

Here we have written $\omega(\alpha)$ for $\omega(\tau(\alpha, t), t)$, $\omega(\alpha')$ for $\omega(\zeta(\alpha', t), t)$, and made use of the fact that $s_\alpha = s_\alpha(t)$ depends on time alone. We have also rewritten the right hand side of Equation (3.14) in terms of θ and s_α. Although the apparent singularity $\zeta = \tau$ is removable, we shall nonetheless discretize (4.6) using spectrally accurate alternate point trapezoidal rule [23],

$$\int_{-\pi}^{\pi} f(\alpha, \alpha')d\alpha' \approx \sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i) \text{ odd}}}^{\frac{N}{2}} f(x_i, x_j)(2h). \tag{4.7}$$

This quadrature rule is normally used for singular integrals but we shall also apply it here for smooth kernels. This is done for convenience (it precludes the need for analytical kernel evaluations at $\alpha = \alpha'$), but more importantly, it allows the use of several important quadrature estimates from [9]. We thus discretize (4.6) as:

$$\omega_i + \frac{\beta h}{\pi i} \sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i)\ \text{odd}}}^{\frac{N}{2}} \left\{ \omega_j^p \left(\frac{S_h \zeta_j}{\zeta_j - \tau_i} - \frac{\overline{S_h \zeta_j}}{\overline{\zeta_j} - \overline{\tau_i}} \right) + \overline{\omega_j^p} \left(\frac{S_h \zeta_j}{\overline{\zeta_j} - \overline{\tau_i}} - \frac{\zeta_j - \tau_i}{(\overline{\zeta_j} - \overline{\tau_i})^2} \overline{S_h \zeta_j} \right) \right\}$$
$$+ \beta(B - iQ)\overline{\tau_i} + 2\beta H_d(t) = -\frac{\chi}{2} \left(\mathcal{S}_i e^{i\theta_i} - \frac{\kappa_B S_h^2 \theta_i}{\sigma^2} i e^{i\theta_i} \right), \tag{4.8}$$

where

$$H_d(t) = \frac{h}{2} \sum_{j=-\frac{N}{2}+1}^{\frac{N}{2}} \omega_j \sigma. \tag{4.9}$$

We note that filtering crucially has been applied to the density ω and its conjugate in the smooth integrands of (4.8) and Equation (4.12), but not to the leading order singular term $\mathcal{H}\omega$. This targeted application of filtering is found to be necessary to make use of parabolic smoothing to prove stability of our method.

We next consider the velocity Equation (3.16). To obtain a stable scheme, a careful treatment of the principal value integrals is required. We first parameterize the integrals by α, then we add and substract the periodic Hilbert transform

$$\mathcal{H}\omega(\alpha) = \frac{1}{2\pi} \text{P.V.} \int_{-\pi}^{\pi} \omega(\alpha') \cot\left(\frac{\alpha - \alpha'}{2} \right) d\alpha', \tag{4.10}$$

from the first integral in Equation (3.16) to obtain:

$$\begin{aligned}
&(u_1 + iu_2)|_\gamma \\
=&\mathcal{H}\omega(\alpha) - \frac{1}{2\pi} \int_{-\pi}^{\pi} \left\{ \omega(\alpha') \left[\frac{\zeta_{\alpha'}(\alpha')}{\zeta(\alpha') - \tau(\alpha)} + \frac{\overline{\zeta_{\alpha'}(\alpha')}}{\overline{\zeta(\alpha')} - \overline{\tau(\alpha)}} + \cot\left(\frac{\alpha - \alpha'}{2} \right) \right] \right. \\
&- \left. \overline{\omega(\alpha')} \left[\frac{\zeta_{\alpha'}(\alpha')}{\overline{\zeta(\alpha')} - \overline{\tau(\alpha)}} - \frac{\zeta(\alpha') - \tau(\alpha)}{(\overline{\zeta(\alpha')} - \overline{\tau(\alpha)})^2} \overline{\zeta_{\alpha'}(\alpha')} \right] \right\} d\alpha' \\
&+ (Q + iB)\overline{\tau} - \frac{iG}{2} \tau.
\end{aligned} \tag{4.11}$$

It is easy to see that the integrand (in curly brackets) in Equation (4.11) is a smooth function of α and α'. This is due to the substraction of the leading order singular part $\mathcal{H}\omega$. The singular integral $\mathcal{H}\omega$ and integral with smooth integrand in Equation (4.11) will be treated differently with regard to filtering, which will be essential in our design of a stable scheme.

The velocity Equation (4.11) can be discretized using alternate point trapezoidal rule as:

$$u_i = \big(u_1 + iu_2\big)_i = \frac{h}{\pi} \sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i)\text{ odd}}}^{\frac{N}{2}} \Big\{\omega_j \cot\Big(\frac{\alpha_i - \alpha_j}{2}\Big) - \omega_j^p G_{ij}^{(1)} + \overline{\omega}_j^p G_{ij}^{(2)}\Big\} + (Q + iB)\overline{\tau}_i - \frac{iG\tau_i}{2}, \tag{4.12}$$

where

$$G_{ij}^{(1)} = \frac{S_h\zeta_j}{\zeta_j - \tau_i} + \frac{\overline{S_h\zeta_j}}{\overline{\zeta_j} - \overline{\tau_i}} + \cot\Big(\frac{\alpha_i - \alpha_j}{2}\Big), \tag{4.13}$$

and

$$G_{ij}^{(2)} = \frac{S_h\zeta_j}{\overline{\zeta_j} - \overline{\tau_i}} - \frac{\zeta_j - \tau_i}{(\overline{\zeta_j} - \overline{\tau_i})^2}\overline{S_h\zeta_j}. \tag{4.14}$$

In the discrete equations, $S_h\tau_i$ can be replaced by $\sigma e^{i\theta_i}$, and similar for $S_h\zeta_j$, (i.e., the application of S_h is not needed here), but for notational convenience, we will continue to use $S_h\tau_i$ to represent the discrete version of τ_α. In our method, we need the discrete normal and tangential velocities,

$$(u_n)_i = -\mathrm{Im}\big\{u_i e^{i\theta_i}\big\}, (u_s)_i = \mathrm{Re}\big\{u_i e^{-i\theta_i}\big\}, \tag{4.15}$$

which follow from Equation (3.17) with $n_i = ie^{i\theta_i}$. Care must be made in the discretization of $u_i e^{i\theta_i}$, for reasons which will become apparent later. We compute $u_i e^{i\theta_i}$ in the following way. Decompose $u_i = \mathcal{H}_h\omega_i + (u_R)_i$, where $\mathcal{H}_h\omega_i$ is the leading order part, and from Equation (4.12)

$$(u_R)_i = \frac{h}{\pi} \sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i)\ \text{odd}}}^{\frac{N}{2}} \Big\{ -\omega_j^p G_{ij}^{(1)} + \overline{\omega}_j^p G_{ij}^{(2)} \Big\} + (Q+iB)\overline{\tau}_i - \frac{iG\tau_i}{2}, \tag{4.16}$$

is the 'remainder'. Then we discretize

$$u_i e^{-i\theta_i} = \mathcal{H}_h(\omega_i e^{-i\theta_i}) - \big[\mathcal{H}_h, e^{-i\theta_i}\big](\omega_i^p) + (u_R)_i e^{-i\theta_i}, \tag{4.17}$$

where $\big[\mathcal{H}_h, e^{-i\theta_i}\big](\omega_i^p)$ is the commutator, defined by

$$\big[\mathcal{H}_h, e^{i\theta_i}\big](\omega_i^p) = \mathcal{H}_h\big(e^{i\theta_i}\omega_i^p\big) - e^{i\theta_i}\mathcal{H}_h\big(\omega_i^p\big). \tag{4.18}$$

It is illustrative to consider the important special case of viscosity matched fluids, for which $\beta = 0$ and $\chi = \frac{1}{2}$. Then the integral or nonlocal term in Equation (4.8) drops out, leading to a considerable simplification. Henceforth, we focus our analysis on this special case, and later generalize for the full problem for arbitrary $0 \le \chi \le 1$ and $-1 \le \beta \le 1$. Taking $\beta = 0$ and $\chi = \frac{1}{2}$ in the discrete equation for ω_i (Equation (4.8)), we see that:

$$\omega_i e^{-i\theta_i} = -\frac{1}{2}\Big(\mathcal{S}_i - i\frac{\kappa_B}{\sigma^2} S_h^2 \theta_i\Big). \tag{4.19}$$

Inserting this into (4.17) and taking the imaginary part per Equation (9.46) gives:

$$(u_n)_i = \frac{\kappa_B}{2\sigma^2}\mathcal{H}_h(S_h^2\theta_i) + \mathrm{Im}\big\{ -\big[\mathcal{H}_h, e^{-i\theta_i}\big](\omega_i^p) + (u_R)_i e^{-i\theta_i}\big\}. \tag{4.20}$$

The significance of the decomposition (4.17) is now apparent: by moving $e^{-i\theta_i}$ into the argument of discrete Hilbert transform, the leading order term of the normal velocity, namely $\frac{\kappa_B}{2\sigma^2}\mathcal{H}(S_h^2\theta_i)$, is linear in θ_i with a spatially constant coefficient that has the right sign to take advantage of parabolic smoothing. This will be critical in energy estimates. We similarly decompose the tangential velocity. Recall that

$(u_s)_i = \text{Re}\{u_i e^{i\theta_i}\}$, then insert Equation (4.19) into Equation (4.17), and take the real part to obtain:

$$(u_s)_i = -\frac{\chi}{2}\mathcal{H}_h(\mathcal{S}_i) + \text{Re}\{ -[\mathcal{H}_h, e^{-i\theta_i}]\omega_i^p + (u_R)_i e^{-i\theta_i}\}. \tag{4.21}$$

We next consider the discretization of the θ and σ equations. The semi-discrete (continuous in time, discrete in space) equations for θ, σ are:

$$\left(\theta_t\right)_i = \frac{1}{\sigma}\left(S_h(u_n)_i + (\phi_s)_i S_h \theta_i\right), \tag{4.22}$$

$$\sigma_t = -\langle u_n S_h \theta \rangle_h, \tag{4.23}$$

where:

$$\langle f \rangle_h = \frac{1}{N} \sum_{j=-\frac{N}{2}+1}^{\frac{N}{2}} f_j, \tag{4.24}$$

is the discrete mean computed using trapezoid rule. In order to recover the interface location from θ_i and σ, we need to introduce the pseudo-spectral antiderivative operator defined in Fourier space on functions f of mean zero by:

$$\left(\widehat{S_h^{-1} f}\right)_k = \begin{cases} \frac{1}{ik}\hat{f}_k & \text{for } k \neq 0, \\ 0 & \text{for } k = 0. \end{cases} \tag{4.25}$$

Then the discretization of Equations (3.30), (3.31) can be written:

$$\tau_i = \tau_c + S_h^{-1}\left(\sigma e^{i\theta} - \langle \sigma e^{i\theta} \rangle_h\right)_i, \tag{4.26}$$

where τ_c is the zero (constant) Fourier mode of τ_i, and is evolved from Equation (3.32) as

$$\frac{d\tau_c}{dt} = \hat{v}_0 = \langle v \rangle_h, \tag{4.27}$$

where $\hat{v}_0$ is the zero Fourier mode of the discrete velocity v_i. Similarly, Equation (3.25) is discretized as:

$$\left(\phi_s\right)_i = S_h^{-1}\left(u_n S_h \theta - \langle u_n S_h \theta \rangle_h\right)_i, \tag{4.28}$$

and the surface tension Equation (3.38) is:

$$\mathcal{S}_i = \frac{\sigma}{\sigma_0 D_h \alpha_{0i}}\left(1 + \mathcal{S}_{0i}\right) - 1, \tag{4.29}$$

where $\mathcal{S}_{0i}$ is the discrete initial tension, and σ_0 is the initial value of s_α. The semi-discrete equation for α_{0i} is obtained from Equation (3.44) as:

$$(\alpha_{0t})_i = \frac{D_h \alpha_{0i}}{\sigma e^{i\theta_i}}\left((\phi_s - u_s)e^{i\theta}\right)_i. \tag{4.30}$$

In summary, the principal equations for discrete scheme are Equations (4.8), (4.20), (4.21), (4.22)-(4.23), (4.26)-(4.30), and are the main result of this chapter.

An example numerical calculation from Higley et al. [22] is shown in Figure 4.1. Their BIM is similar, but not identical to, that described in this chapter. In particular, the BIM given in this chapter generalizes that of [22] to include nonzero interior viscosity and membrane bending stress. Numerical results using the method given in this chapter will be presented in later work.

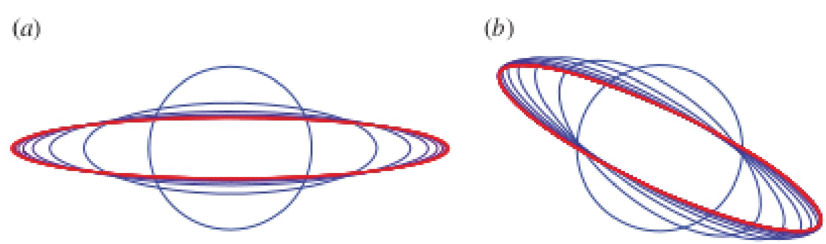

Figure 4.1 The time evolution of a capsule in (a) a pure strain flow and (b) a simple shear flow with $\mathcal{S}_0 = 1$. The capsule profiles are shown at intervals of (a) $\Delta t = 1.0$ and (b) $\Delta t = 0.5$.
Source [22].

CHAPTER 5

PRELIMINARY LEMMAS

We define the Sobolev norm in a general region $\Omega \subset \mathbb{R}^d$ as follows:

$$\|u\|_{W^{m,p}(\Omega)} = \left(\sum_{|\alpha| \leq m} \|D^\alpha u\|^p_{L^p(\Omega)} \right)^{\frac{1}{p}}. \tag{5.1}$$

Another equivalent definition, with respect to the Fourier transform $\mathcal{F}$, is:

$$\|u\|_{W^{m,p}(\Omega)} = \left\| \mathcal{F}^{-1}\left[\left(1 + |k|^2\right)^{\frac{m}{2}} \mathcal{F}(u) \right] \right\|_{L^p(\Omega)}. \tag{5.2}$$

A particular Sobolev space, which we use in this paper is $H^s = W^{s,2}$, defined by the following:

$$\|f\|_s = \left(\sum_{k=-\infty}^{\infty} \left(1 + |k|^2\right)^s |\hat{f}_k|^2 \right)^{\frac{1}{2}}. \tag{5.3}$$

The subsequent analysis makes use of the Sobolev embedding theorem:

Theorem 5.0.1. *If $m \geq l$ and $m - \frac{d}{p} \geq l - \frac{d}{q}$, then $W^{m,p}(\Omega) \subset W^{l,q}(\Omega)$.*

This theorem can be found in [1].

The first lemma gives the accuracy of the pseudo spectral derivative.

Lemma 5.0.2. *(see [18]) Let $f(\alpha)$ be a periodic $C^{s+1}[-\pi, \pi]$ function. Then:*

$$|S_h f(\alpha_i) - f_\alpha(\alpha_i)| \leq c h^{s-\frac{1}{2}} \|f\|_{s+1}. \tag{5.4}$$

The same inequality holds for D_h in place of S_h.

Proof. Let $\hat{f}^e_k$ to be the exact Fourier coefficient of f. Then:

$$\hat{f}_k = \hat{f}^e_k + \sum_{j \neq 0} \hat{f}^e_{k+Nj}, \text{ for } k = -\frac{N}{2} + 1, \cdots, \frac{N}{2}, \tag{5.5}$$

(see [18], section 5) is the computed coefficient from Equation (4.3), where the sum represents 'high wave numbers' modes (i.e., those with $|k| > \frac{N}{2}$) that are aliased to $k \in \left[-\frac{N}{2}+1, \frac{N}{2}\right]$. Introduce the notation $|k| \leq \frac{N'}{2}$ defined as $\left\{k : -\frac{N}{2}+1 \leq k \leq \frac{N}{2}\right\}$ and similarly the notation $|k| > \frac{N'}{2}$ is defined as $\left\{k : \frac{N}{2} < k \text{ or } k \leq -\frac{N}{2}\right\}$. Then we have the estimate

$$
\begin{aligned}
|S_h f(\alpha_i) - f_\alpha(\alpha_i)| &= \left| \sum_{|k| \leq \frac{N'}{2}} \left(\left(\widehat{f_\alpha}\right)_k - \left(\widehat{f_\alpha}\right)^e_k \right) e^{ik\alpha_i} - \sum_{|k| > \frac{N'}{2}} \left(\widehat{f_\alpha}\right)^e_k e^{ik\alpha_i} \right| \\
&\leq \left| \sum_{|k| \leq \frac{N'}{2}} k(\hat{f}_k - \hat{f}^e_k) e^{ik\alpha_i} \right| + \left| \sum_{|k| > \frac{N'}{2}} k \hat{f}^e_k e^{ik\alpha_i} \right| \\
&\leq \sum_{|k| \leq \frac{N'}{2}} |k| |\hat{f}_k - \hat{f}^e_k| + \sum_{|k| > \frac{N'}{2}} |k| |\hat{f}^e_k|.
\end{aligned} \tag{5.6}
$$

The first term on the right hand of (5.6) is the aliasing error, and the second term is the truncation error. We use Equation (5.5) to bound the aliasing error as follows:

$$
\begin{aligned}
\sum_{|k| \leq \frac{N'}{2}} |k| |\hat{f}_k - \hat{f}^e_k| &= \sum_{|k| \leq \frac{N'}{2}} |k| \left| \sum_{j \neq 0} \hat{f}^e_{k+Nj} \right| \\
&\leq \sum_{\substack{|k| \leq \frac{N'}{2} \\ j \neq 0}} |k + jN| |\hat{f}^e_{k+Nj}| \leq \sum_{|\tilde{k}| \geq \frac{N}{2}} |\tilde{k}| |\hat{f}^e_{\tilde{k}}|,
\end{aligned} \tag{5.7}
$$

where $\tilde{k} = k + jN$, with $j \neq 0$. The last line of (5.7) follows from

$$
|\tilde{k}| = |k + jN| \geq \big| |k| - j|N| \big| \geq \left| \frac{N}{2} - N \right| \geq \frac{N}{2}. \tag{5.8}
$$

Then this aliasing error is further bounded by (dropping the tilde):

$$\begin{aligned}
\sum_{|k|\ge\frac{N}{2}} |k||\hat{f}_k^e| &\le \sum_{|k|\ge\frac{N}{2}} \frac{|k|^{s+1}}{|k|^s}|\hat{f}_k^e|, \\
&\le \Big(\sum_{|k|\ge\frac{N}{2}} |k|^{2(s+1)}|\hat{f}_k^e|^2\Big)^{\frac{1}{2}}\Big(\sum_{|k|\ge\frac{N}{2}} \frac{1}{|k|^{2s}}\Big)^{\frac{1}{2}}, \text{ using Cauchy-Schwartz} \\
&\le c\|f\|_{H^{s+1}}\big(N^{-2s+1}\big)^{\frac{1}{2}}, \\
&\le ch^{s-\frac{1}{2}}\|f\|_{s+1}, \text{ using } h = \frac{2\pi}{N}.
\end{aligned} \tag{5.9}$$

Here we have used the bound:

$$\sum_{|k|\ge\frac{N}{2}} \frac{1}{|k|^{2s}} < cN^{-2s+1}, \tag{5.10}$$

which follow from the integral test:

$$\int_{\frac{N}{2}}^{\infty} x^{-2s}dx \sim \left(\frac{x^{-2s+1}}{-2s+1}\right)\Big|_{\frac{N}{2}}^{\infty} = cN^{-2s+1}. \tag{5.11}$$

The truncation error term is bounded as (starting from Equation (5.6)):

$$\begin{aligned}
\sum_{|k|>\frac{N'}{2}} |k||\hat{f}_k^e| &= \sum_{|k|>\frac{N'}{2}} \frac{|k|^{s+1}}{|k|^s}|\hat{f}_k^e|, \\
&\le \Big(\sum_{|k|>\frac{N'}{2}} |k|^{2(s+1)}|\hat{f}_k^e|^2\Big)^{\frac{1}{2}}\Big(\sum_{|k|>\frac{N'}{2}} |k|^{-2s}\Big)^{\frac{1}{2}}, \text{ by Cauchy-Schwartz} \\
&\le ch^{s-\frac{1}{2}}\|f\|_{s+1}.
\end{aligned} \tag{5.12}$$

Combine the estimates of aliasing error and truncation error to obtain:

$$|S_h f(\alpha_i) - f_\alpha(\alpha_i)| \le ch^{s-\frac{1}{2}}\|f\|_{s+1}. \tag{5.13}$$

The proof of (5.13) for D_h instead of S_h is similar. □

The next lemma is a well-known result on the accuracy of trapezoid rule for periodic functions.

Lemma 5.0.3. *Let $f(\alpha)$ be as in Lemma 5.0.2. Then:*

$$\left| \sum_{j=-\frac{N}{2}+1}^{\frac{N}{2}} f(\alpha_j)h - \int_{-\pi}^{\pi} f(\alpha)d\alpha \right| \leq ch^{s+1}\|f\|_{s+1}. \tag{5.14}$$

Proof. This is derived from the Euler−Maclaurin formula. For more details, see [21]. □

Similarly for the pseudo−spectral integral operator we have:

Lemma 5.0.4. *Let f be a periodic, zero−mean, $C^s[-\pi, \pi]$ function. Then:*

$$\left|\partial_\alpha^{-1} f(\alpha_j) - S_h^{-1} f(\alpha_j)\right| \leq ch^{s-\frac{1}{2}}\|f\|_s. \tag{5.15}$$

Proof. We estimate from Equation (4.25):

$$\begin{aligned}
&\left|\partial_\alpha^{-1} f(\alpha_j) - S_h^{-1} f(\alpha_j)\right| \\
=&\left| \sum_{k=-\infty}^{\infty} \frac{\hat{f}_k^e e^{ik\alpha_i}}{ik} - \sum_{|k|\leq \frac{N'}{2}} \frac{\hat{f}_k e^{ik\alpha_i}}{ik} \right| \\
=&\left| \sum_{|k|>\frac{N'}{2}} \frac{\hat{f}_k^e e^{ik\alpha_i}}{ik} - \sum_{|k|\leq \frac{N'}{2}} \sum_{j\neq 0} \frac{\hat{f}_{k+Nj}^e e^{ik\alpha_i}}{ik} \right| \\
\leq&\left(\sum_{|k|>\frac{N'}{2}} \frac{|\hat{f}_k^e|}{|k|} + \sum_{|k|\leq \frac{N'}{2}} \frac{1}{|k|} \sum_{j\neq 0} |\hat{f}_{k+jN}^e| \right),
\end{aligned} \tag{5.16}$$

where we have used Equation (5.5) in the second equality. The first term in (5.16) corresponds to the truncation error, and the second term to the aliasing error.

Then the aliasing error is bounded by:

$$\begin{aligned}
&\sum_{|k|\le \frac{N'}{2}} \frac{1}{|k|} \sum_{j\neq 0} |\hat{f}^e_{k+jN}| \le \sum_{|k|\le \frac{N'}{2}} \sum_{j\neq 0} |\hat{f}^e_{k+jN}|, \\
&\le \sum_{|k|\ge \frac{N}{2}} |\hat{f}^e_k| = \sum_{|k|\ge \frac{N}{2}} \frac{|k|^s}{|k|^s} |\hat{f}^e_k|, \text{ by Equation (5.8)} \\
&\le \Big(\sum_{|k|\ge \frac{N}{2}} |k|^{2s} |\hat{f}^e_k|^2 \Big)^{\frac{1}{2}} \Big(\sum_{|k|\ge \frac{N}{2}} \frac{1}{|k|^{2s}} \Big)^{\frac{1}{2}}, \text{ by Cauchy-Schwartz} \\
&\le c \Big(\sum_{|k|\ge \frac{N}{2}} |k|^{2s} |\hat{f}^e_k|^2 \Big)^{\frac{1}{2}} N^{\frac{-2s+1}{2}}, \\
&\le c h^{s-\frac{1}{2}} \|f\|_s, \qquad (5.17)
\end{aligned}$$

and the truncation error is bounded by:

$$\begin{aligned}
&\sum_{|k| > \frac{N'}{2}} \frac{|\hat{f}^e_k|}{|k|} = \sum_{|k| > \frac{N'}{2}} \frac{|k|^s}{|k|^{s+1}} |\hat{f}^e_k|, \\
&\le \Big(\sum_{|k| > \frac{N'}{2}} |k|^{2s} |\hat{f}^e_k|^2 \Big)^{\frac{1}{2}} \Big(\sum_{|k| > \frac{N'}{2}} \frac{1}{|k|^{2(s+1)}} \Big)^{\frac{1}{2}}, \text{ by Cauchy-Schwartz} \\
&\le c \Big(\sum_{|k| > \frac{N'}{2}} |k|^{2s} |\hat{f}^e_k|^2 \Big)^{\frac{1}{2}} N^{\frac{-2(s+1)+1}{2}}, \\
&\le c \|f\|_s h^{\frac{2s+1}{2}} = c h^{s+\frac{1}{2}} \|f\|_s. \qquad (5.18)
\end{aligned}$$

Thus, the total error is bounded by:

$$\left| \partial_\alpha^{-1} f(\alpha_j) - S_h^{-1} f(\alpha_j) \right| \le c h^{s-\frac{1}{2}} \|f\|_s. \qquad (5.19)$$

□

The next lemma provides a result on the accuracy of the pseudospectral smoothing of f.

Lemma 5.0.5. *Let $f \in C^s[-\pi, \pi]$ be periodic, and let f^p be as defined in Equation (4.4) with conditions (i)–(iv). Then:*

$$|f^p(\alpha_i) - f(\alpha_i)| \le ch^{s-\frac{1}{2}} \|f\|_s. \tag{5.20}$$

Proof. The proof is similar to that for Lemma 5.0.2, and is omitted here. □

Remark 5.0.6. *Due to the asymmetry of the discrete Fourier transform, we will zero out the $k = \frac{N}{2}$ mode of $(\widehat{S_h f})_k$. This will be important for utilizing the smoothing properties of the highest derivative term. It is easy to see that zeroing out this mode does not affect any of the estimates in this chapter.*

CHAPTER 6

CONSISTENCY

We calculate the error when the exact solution is substituted into the discrete system of equations. Assume the exact solution is regular enough so that $\theta(\cdot,t) \in C^{m+1}[-\pi,\pi]$, $\omega(\cdot,t) \in C^{m-1}[-\pi,\pi]$ and $\alpha_0(\cdot,t) \in C^{m+1}[-\pi,\pi]$. We also assume the initial tension $\mathcal{S}(\cdot,0)$ is in $C^m[-\pi,\pi]$. The different levels of regularity for the different functions follows from an analysis of the continuous evolution equations. We denote by $u_h(\alpha_i)$, $(u_n)_h(\alpha_i)$, $(\phi_s)_h(\alpha_i)$, etc. quantities that are evaluated by substituting the exact solutions $\omega(\cdot,t), \theta(\cdot,t), s_\alpha(t)$ into the discrete equations. We make repeated use of the estimate

$$\tau_h(\alpha_i) = \tau_c + S_h^{-1}\big(s_\alpha e^{i\theta} - \langle s_\alpha e^{i\theta}\rangle_h\big)(\alpha_i) = \tau(\alpha_i) + \mathrm{O}(h^{m+\frac{1}{2}}). \tag{6.1}$$

which follows from Equation (4.26), Lemma 5.0.4, and the assumption on the regularity of the exact solution.

Consistency of ω equation:

We first assess the smoothness of the integrand in the continuous equation for ω, Equation (4.6). Let $F(\alpha,\alpha')$ denote the integrand (terms in brackets) in Equation (4.6). We note that by Lemma 5.0.5, the filtered density ω^p can be replaced by an unfiltered ω, incurring an $\mathrm{O}(h^{m-\frac{3}{2}})$ error based on the regularity of $F(\alpha,\alpha')$ (see Equation (6.3)). Now, the apparent singularity in $F(\alpha,\alpha')$ is removable, and

$$\lim_{\alpha'\to\alpha} F(\alpha,\alpha') = i\Big(\omega(\alpha)\kappa(\alpha)s_\alpha + \frac{\overline{\omega}(\alpha)\kappa(\alpha)\tau_\alpha^2(\alpha)}{s_\alpha}\Big). \tag{6.2}$$

Recalling that $\omega(\cdot) \in C^{m-1}$, $\tau_\alpha(\cdot) = s_\alpha e^{i\theta(\cdot)} \in C^{m+1}$, and that s_α is bounded away from zero, it follows that:

$$F(\alpha, \cdot) \in C^{m-1}. \tag{6.3}$$

Now consider the discrete sum in Equation (4.8) with integrand $F = F_h$, where the subscript h denotes its evaluation using $\tau = \tau_h$, $\zeta = \zeta_h$, and the exact ω. By Equation (6.1), we can replace $\tau_h(\alpha_i)$ and $\zeta_h(\alpha_j)$ in this sum by $\tau(\alpha_i)$ (respectively $\zeta(\alpha_j)$), incurring an order $\mathrm{O}(h^{m+\frac{1}{2}})\big[\min_j \big(\zeta(\alpha_j) - \tau(\alpha_i)\big)\big]^{-1} = \mathrm{O}(h^{m-\frac{1}{2}})$ error. There is no error in $S_h(\zeta(\alpha_j))$ since the exact solution $s_\alpha e^{i\theta(\alpha_i)}$ is substituted for this term. We compute the truncation error of the alternate point trapezoidal rule sum in Equation (4.8). Let

$$\begin{aligned} J_h(\alpha_i) &= \sum_{j=-\frac{N}{2}+1}^{\frac{N}{2}} F_h(\alpha_i, \alpha_j)h \\ &= \sum_{j=-\frac{N}{2}+1}^{\frac{N}{2}} F(\alpha_i, \alpha_j)h + \mathrm{O}(h^{m-\frac{1}{2}}), \end{aligned} \tag{6.4}$$

where we have used the above remarks to replace F_h with F, and define the truncation error

$$J_h^e(\alpha_i) = J_h(\alpha_i) - \int_{-\pi}^{\pi} F(\alpha_i, \alpha')d\alpha'. \tag{6.5}$$

Then by the error estimate for trapezoidal rule integration (Lemma 5.0.3), we have:

$$\big|J_h^e(\alpha_i)\big| \leq ch^{m-1}\|F(\alpha_i, \cdot)\|_{m-1} = \mathrm{O}(h^{m-1}). \tag{6.6}$$

Note that if i is even,

$$
\begin{aligned}
&2J_h^e(\alpha_i) - J_{2h}^e(\alpha_i) \\
=&2\sum_{j=-\frac{N}{2}+1}^{\frac{N}{2}} F_h(\alpha_i, \alpha_j)h - \sum_{j=-\frac{N}{4}+1}^{\frac{N}{4}} F_h(\alpha_i, \alpha_{2j})2h - \int_{-\pi}^{\pi} F_h(\alpha_i, \alpha')d\alpha', \\
=&\sum_{\substack{j=-\frac{N}{2}+1 \\ j \text{ odd}}}^{\frac{N}{2}} F_h(\alpha_i, \alpha_j)2h - \int_{-\pi}^{\pi} F(\alpha_i, \alpha')d\alpha', \qquad (6.7)
\end{aligned}
$$

which together with Equation (6.6) implies:

$$
\sum_{\substack{j=-\frac{N}{2}+1 \\ j \text{ odd}}}^{\frac{N}{2}} F_h(\alpha_i, \alpha_j)2h - \int_{-\pi}^{\pi} F(\alpha_i, \alpha')d\alpha' = \mathrm{O}(h^{m-1}). \qquad (6.8)
$$

A similar argument shows that if i is odd

$$
\sum_{\substack{j=-\frac{N}{2} \\ j \text{ even}}}^{\frac{N}{2}} F_h(\alpha_i, \alpha_j)2h - \int_{-\pi}^{\pi} F(\alpha_i, \alpha')d\alpha' = \mathrm{O}(h^{m-1}). \qquad (6.9)
$$

Equations (6.8) and (6.9) can be combined into

$$
\sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i) \text{ odd}}}^{\frac{N}{2}} F_h(\alpha_i, \alpha_j)2h - \int_{-\pi}^{\pi} F(\alpha_i, \alpha')d\alpha' = \mathrm{O}(h^{m-1}), \qquad (6.10)
$$

which gives the truncation error for the alternate point trapezoidal rule quadrature in Equation (4.8). Error estimates for other terms in the discrete ω equation are obtained using Lemma 5.0.2. For example, the last term in Equation (4.8) satisfies:

$$
\left| \frac{S_h^2\theta(\alpha_i)}{s_\alpha^2} - \frac{\theta_{\alpha\alpha}(\alpha_i)}{s_\alpha^2} \right| = \mathrm{O}(h^{m-\frac{5}{2}}), \qquad (6.11)
$$

where we have used that $\tau_\alpha(\cdot)$ is in $C^{m+1}[-\pi,\pi]$. The other terms are found to have higher-order error in h. It follows that:

$$\omega(\alpha_i)+\frac{\beta}{2\pi i}\sum_{\substack{j=-\frac{N}{2}\\(j-i)\text{ odd}}}^{\frac{N}{2}} F_h(\alpha_i,\alpha_j)2h+\beta(B-iQ)\overline{\tau_h(\alpha_i)}+\beta h\sum_{j=1}^{N}\omega(\alpha_j)|S_h\tau_h(\alpha_i)|$$
$$+\frac{\chi}{2}\Big(\mathcal{S}_h(\alpha_i)-\mathcal{S}(\alpha_i)-i\frac{\kappa_B}{s_\alpha^2}\big(S_h^2\theta(\alpha_i)-\theta_{\alpha\alpha}(\alpha_i)\big)\Big)e^{i\theta(\alpha_i)}=\mathrm{O}(h^{m-\frac{5}{2}}),\quad (6.12)$$

which shows the consistency of the discrete scheme Equation (4.8).

Remark 6.0.1. *When $\beta=0$ and $\chi=\frac{1}{2}$, Equation (4.8) provides an expect relation for ω_i in terms of θ_i, σ and $\mathcal{S}_i$. Let $\omega_h(\alpha_i)$ denote the quantity obtained by substituting the exact solution $\theta(\cdot,t)$, $s_\alpha(t)$ and $\mathcal{S}(\cdot,t)$ into Equation (4.8). Then the above remarks show that:*

$$\omega_h(\alpha_i)=\omega(\alpha_i)+O(h^{\frac{5}{2}}) \quad (6.13)$$

Consistency of velocity:

Let $G(\alpha,\alpha')$ be the integrand (quantity in curly brackets) in Equation (4.11). We once again use Lemma 5.0.5 to replace the filtered ω^p with unfiltered ω, incurring an $\mathrm{O}(h^{m-\frac{3}{2}})$ error per the regularity of G given below. Then:

$$\lim_{\alpha'\to\alpha} G(\alpha,\alpha')=-\omega(\alpha)\mathrm{Re}\Big(\frac{\tau_{\alpha\alpha}}{\tau_\alpha}\Big)+i\overline{\omega(\alpha)}\kappa(\alpha)\frac{\tau_\alpha^2(\alpha)}{s_\alpha}, \quad (6.14)$$

and it follows that $G(\alpha,\cdot)\in C^{m-1}$. Using the same argument as that which led to Equation (6.10), we deduce the quadrature error,

$$\sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\text{ odd}}}^{\frac{N}{2}} G_h(\alpha_i,\alpha_j)2h-\int_{-\pi}^{\pi}G(\alpha_i,\alpha')d\alpha'=\mathrm{O}(h^{m-1}), \quad (6.15)$$

Let:

$$\mathcal{H}_h\omega(\alpha_i) = \frac{1}{2\pi} \sum_{\substack{j=-\frac{N}{2} \\ (j-i)\ \text{odd}}}^{\frac{N}{2}} \omega(\alpha_j) \cot\Big(\frac{\alpha_i - \alpha_j}{2}\Big) 2h \tag{6.16}$$

denote the discrete Hilbert transform. Then it is shown in [9] that:

$$\Big| \mathcal{H}_h\omega(\alpha_i) - \frac{1}{2\pi}\text{P.V.} \int_{-\pi}^{\pi} \omega(\alpha') \cot\Big(\frac{\alpha - \alpha'}{2}\Big) d\alpha' \Big| = \text{O}(h^{m-2}). \tag{6.17}$$

This is a special case of a result proven in Chapter 2 of [9], where it is shown that the order of accuracy of the quadrature in (6.16) is related to the regularity of $\omega_\alpha(\cdot)$ which here is C^{m-2}. It follows that

$$\begin{aligned} u_h(\alpha_i) = \mathcal{H}_h\omega(\alpha_i) - \frac{1}{2\pi} \sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i)\ \text{odd}}}^{\frac{N}{2}} G_h(\alpha_i, \alpha_j) 2h + (Q + iB)\tau_h(\alpha_i) \\ - \frac{iG\tau_h(\alpha_i)}{2} = u(\alpha_i) + \text{O}(h^{m-2}), \end{aligned} \tag{6.18}$$

which shows the consistency of Equation (4.12). From this it is easy to see that,

$$(u_s)_h(\alpha_i) = u_s(\alpha_i) + \text{O}(h^{m-2}), \text{ and} \tag{6.19}$$

$$(u_n)_h(\alpha_i) = u_n(\alpha_i) + \text{O}(h^{m-2}), \tag{6.20}$$

$$S_h(u_n)_h(\alpha_i) = S_h(u_n + \text{O}(h^{m-2}))(\alpha_i) = (u_n)_\alpha(\alpha_i) + \text{O}(h^{m-3}). \tag{6.21}$$

We note that a better estimate (i.e., one with higher order error) can be obtained for $(u_s)_h$, but (6.19) will be sufficient for our purposes. In addition, from Equation (4.26),

$$(\phi_s)_h(\alpha_i) = S_h^{-1}\big((u_n)_h S_h\theta - \langle (u_n)_h S_h\theta \rangle_h\big)(\alpha_i) = \phi_s(\alpha_i) + \text{O}(h^{m-2}), \tag{6.22}$$

with the latter equality follows from Lemmas 5.0.3-5.0.4, (6.20), and $u_n(\cdot) \in C^{m-1}$. In particular, note that the leading source of error in (6.21) and (6.22) comes from the $\mathrm{O}(h^{m-2})$ term in Equation (6.20). Combined, the above results show that the truncation errors for the $\theta, s_\alpha, \alpha_0$ evolution Equations (4.22)-(4.23), (4.30) are given by

$$\frac{\partial}{\partial t}\theta(\alpha_i) = \frac{1}{s_\alpha}\big[S_h(u_n)_h(\alpha_i) + S_h\theta(\alpha_i)(\phi_s)_h(\alpha_i)\big] + \mathrm{O}(h^{m-3}), \tag{6.23}$$

$$\frac{\partial}{\partial t}s_\alpha = -\langle (u_n)_h(\cdot)S_h\theta(\cdot)\rangle_h + \mathrm{O}(h^{m-2}), \tag{6.24}$$

$$\frac{\partial \alpha_0}{\partial t}(\alpha_i) = \frac{S_h\alpha_0(\alpha_i)}{s_\alpha e^{i\theta(\alpha_i)}}\big((u_n)_h i e^{i\theta} + (\phi_s)_h e^{i\theta} - u_h\big)(\alpha_i) + \mathrm{O}(h^{m-2}). \tag{6.25}$$

We also need to check consistency of the discrete version of kinematic condition (Equation (3.20)). Differentiate Equation (4.26) with respect to t to obtain:

$$\frac{d\tau_i}{dt} = \frac{d\tau_c}{dt} + S_h^{-1}\Big(\frac{d\sigma}{dt}e^{i\theta} + i\sigma e^{i\theta}\frac{d\theta}{dt} - \langle \frac{d\sigma}{dt}e^{i\theta} + i\sigma e^{i\theta}\frac{d\theta}{dt}\rangle_h\Big)_i, \tag{6.26}$$

where from Equation (4.27),

$$\frac{d\tau_c}{dt} = \langle v\rangle_h. \tag{6.27}$$

Then it is easy to see that:

$$\frac{d\tau}{dt}(\alpha_i) = \frac{d\tau_h}{dt}(\alpha_i) + \mathrm{O}(h^{m-3}). \tag{6.28}$$

Taken together, the above results prove the following consistency result:

Lemma 6.0.2. *Under the assumption that $\theta(\cdot,t)$ and $\alpha_0(\cdot,t)$ are in $C^{m+1}[-\pi,\pi]$, $\mathcal{S}_0(\cdot)$ is in $C^m[-\pi,\pi]$, and $\omega(\cdot,t)$ is in $C^{m-1}[-\pi,\pi]$, the exact solution of the evolution equations satisfy the discrete equations with a truncation error at most of size $O(h^{m-3})$.*

CHAPTER 7

STATEMENT OF MAIN CONVERGENCE THEOREM

To show convergence of the numerical method, we need to establish the stability of the discrete scheme. We first do this for special case of viscosity matched fluids, for which $\beta = 0$ and $\chi = \frac{1}{2}$. Define the errors between the exact and numerical solutions as:

$$\begin{aligned} \dot{\theta}_j &= \theta_j - \theta(\alpha_j), \\ \dot{\omega}_j &= \omega_j - \omega_h(\alpha_j), \\ \dot{u}_j &= u_j - u_h(\alpha_j), \end{aligned} \tag{7.1}$$

and so forth. To show stability, we plan to obtain a system of evolution equations for these errors and perform energy estimates to show they remain bounded for $t \leq T$, where T is the assumed existence time for an exact solution to the continuous problem.

To illustrate this idea, let us find an equation for $\dot{\theta}$. First, substitute the exact solution into Equations (6.23)−(6.24) and use the consistency lemma to get:

$$\begin{aligned} \frac{d\dot{\theta}_i}{dt} &= \frac{1}{\sigma_i}\big[S_h(u_n)_i + S_h\theta_i(\phi_s)_i\big] \\ &- \frac{1}{\sigma_h}\big[S_h(u_n)_h(\alpha_i) + S_h\theta(\alpha_i)(\phi_s)_h(\alpha_i)\big] + \mathrm{O}(h^{m-3}) \\ \frac{d\dot{\sigma}_i}{dt} &= S_h(\phi_s)_i + (S_h\theta_i)(u_n)_i \\ &- \big[S_h(\phi_s)_h(\alpha_i) + S_h\theta(\alpha_i)(u_n)_h(\alpha_i)\big] + \mathrm{O}(h^{m-2}) \\ &= -\langle (u_n)S_h(\theta(\cdot))\rangle_i + \langle (u_n)_h(\alpha_i)S_h(\theta(\alpha_i))\rangle_h + \mathrm{O}(h^{m-2}). \end{aligned} \tag{7.2}$$

Now, the right hand side of the above equation can be written in terms of $\dot{\theta}_i, \dot{s}_\alpha$, and the variations in velocities:

$$(\dot{u_n})_i = (u_n)_i - (u_n)_h(\alpha_i),\ (\dot{\phi_s})_i = (\phi_s)_i - (\phi_s)_h(\alpha_i). \tag{7.3}$$

Therefore, our first task is to estimate quantities such as $(\dot{u_n})_i$ and $(\dot{\phi_s})_i$ in terms of the errors $\dot{\theta}_i, \dot{\sigma}_i$. This can be done by identifying the most singular part in the variation $\dot{u}_i = u_i - u_h(\alpha_i)$ of the complex velocity. The estimates can be separated into linear and nonlinear terms in $\dot{\theta}_i, \dot{\sigma}_i$. The nonlinear terms can be controlled by the high accuracy of the method for smooth solutions. Thus the leading order error contribution comes from the linear terms.

Remark 7.0.1. *If $\dot{\phi}$ is a scalar quantity, we will sometimes use the notation $O(\dot{\phi})$ to denote a bounded operator in l^2, i.e.,*

$$\|O(\dot{\phi})\|_{l^2} \leq c|\dot{\phi}|. \tag{7.4}$$

Thus, $O(\dot{\phi})$ is equivalent to $A_0(\dot{\phi})$. For example, if $f(\cdot) \in C[-\pi, \pi]$, then $f(\alpha_i)(\dot{\phi}) = O(\dot{\phi})$.

We now state the convergence theorem for our numerical method:

Theorem 7.0.2. *Assume that for $0 \leq t \leq T$, there exist a smooth solution of the continuous problem (Equations (3.22)–(3.23), (3.20), (4.30)) with $\theta(\cdot, t)$, $\alpha_0(\cdot, t)$ in $C^{m+1}[-\pi, \pi]$ and $\mathcal{S}(\cdot, 0) \in C^m[-\pi, \pi]$ for m sufficiently large, and that:*

$$\min_{0 \leq t \leq T} s_\alpha(t) > c, \text{ for some } c > 0. \tag{7.5}$$

If σ_h and θ_h denote the numerical solution for s_α, θ, then for h sufficiently small:

$$\begin{aligned} \|\sigma_h(t) - s_\alpha(t)\|_{l^2} &\leq c(T)h^s, \\ \|\theta_h(t) - \theta(\cdot, t)\|_{l^2} &\leq c(T)h^s, \\ \|\tau_h(t) - \tau(\cdot, t)\|_{l^2} &\leq c(T)h^s, \\ \|(\alpha_0)_h(t) - \alpha_0(\cdot, t)\|_{l^2} &\leq c(T)h^s, \end{aligned} \tag{7.6}$$

where $s = m + 1 - l$ *and* $0 \leq l \leq m$ *is small positive integer that is independent of* m*(i.e.,* s *is near* m*). Here:*

$$\|u\|_{l^2} = h \sum_{j=-\frac{N}{2}+1}^{\frac{N}{2}} |u_j|^2. \tag{7.7}$$

CHAPTER 8

STABILITY: PRELIMINARIES

Following [13] and [9], we introduce an n-th order smoothing operator A_{-n} which satisfies:

$$\|D_h^k(A_{-n}(\dot{\phi}_j))\|_{l^2} \leq c\|\dot{\phi}\|_{l^2} \text{ and } \|A_{-n}(S_h^k(\dot{\phi}_j))\|_{l^2} \quad \leq c\|\dot{\phi}\|_{l^2} \text{ for } 0 \leq k \leq n. \tag{8.1}$$

where D_h is the spectral derivative operator with smoothing. When $n = 0$, $A_0(\dot{\phi})$ denotes a bounded operator in l^2,

$$\|A_0(\dot{\phi}_j)\|_{l^2} \leq c\|\dot{\phi}\|_{l^2}. \tag{8.2}$$

Remark 8.0.1. *Note that if $f(\dot{\phi}_i) = A_0(\dot{\phi}_i)$, then $h^s f(\dot{\phi}_i) = A_{-s}(\dot{\phi}_i)$. However, $f(\dot{\phi}_i) = A_{-s}(\dot{\phi}_i)$ does not imply $f = O(h^s)$. An example is $f(\dot{\phi}_i) = 1 + h^s\dot{\phi}_i$, which is an $A_{-s}(\dot{\phi}_i)$, but not $O(h^s)$.*

Remark 8.0.2. *We use the expression $A_{-s}(\dot{\phi}_i)$ to denote a generic high$-$order smoothing operator. Generally, s will be an integer near m, e.g., $m+1$ or $m-1$, where m gives the regularity of the continuous solution (i.e., $\theta(\cdot, t) \in C^{m+1}$, etc.). Similarly, we use the expression $O(h^s)$ to denote a high order discretization error, again where s is near m. At the end of our proof, we may choose m and s large enough, so that all the estimates go through.*

Remark 8.0.3. *Unless otherwise noted, we use the phrase "smooth function" to denote a generic function $f \in C^s[-\pi, \pi]$ with high order regularity.*

Remark 8.0.4. *We sometimes will use the notation $A_{-s}(\dot{\phi}_i, \dot{\psi}_i, \ldots, \dot{\omega}_i) = A_{-s}(\dot{\phi}_i) + A_{-s}(\dot{\psi}_i) + \ldots + A_{-s}(\dot{\omega}_i)$.*

We first recall that we have defined a time:

$$T^* \equiv \sup \left\{ t : 0 \leq t \leq T, \|\dot{\sigma}\|_{l^2}, \|\dot{\theta}\|_{l^2}, \|\dot{\zeta}\|_{l^2}, \|\dot{\alpha_0}\|_{l^2} \leq h^{\frac{7}{2}} \right\}. \tag{8.3}$$

The power of h in the above definition is chosen for convenience, so that the estimates below easily go through. All the estimates we obtain are valid for $t \leq T^*$. We "close the argument" and prove Theorem 7.0.2 by showing at the end that $T^* = T$. We make repeated use of the inequalities:

$$\|\dot{\theta}\|_\infty \leq h^3, \ \|\dot{\sigma}\|_\infty \leq h^3, \text{ and } \|\dot{\alpha_0}\|_\infty \leq h^3, \text{ for } t \leq T^* \tag{8.4}$$

The above estimate on $\dot{\theta}$ follows from $h|\dot{\theta}_i|^2 \leq \|\dot{\theta}\|_{l^2}^2$, for $t \leq T^*$, so that $\|\dot{\theta}\|_\infty \leq h^{-\frac{1}{2}} \|\dot{\theta}\|_{l^2} \leq h^3$, with similar estimates applying to $\|\dot{\sigma}\|_\infty$ and $\|\dot{\alpha_0}\|_\infty$.

Preliminary Lemmas:

We state a number of preliminary lemmas that will be repeatedly used in the analysis.

First, we will frequently encounter a discrete operator of the form:

$$R_h(\phi_i) = \sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i) \text{ odd}}}^{\frac{N}{2}} f(\alpha_i, \alpha_j)\phi_j(2h), \tag{8.5}$$

where $f(\alpha, \alpha')$ is a smooth periodic function in both variables, and ϕ is a generic periodic function. Beale, Hou and Lowengrub [9] prove the following estimate on R_h applied to a filtered discrete function ϕ_i^p.

Lemma 8.0.5. *Assume $f(\alpha, \alpha')$ is a smooth periodic function in both α and α', with $f(\cdot_1, \cdot_2) \in C^r$ for $r > 2$, then R_h defined in Equation (8.5) satisfies:*

$$R_h(\phi^p) = A_{-1}(\phi). \tag{8.6}$$

If, in addition, $\rho(x)$ satisfies $\rho'(\pm\pi) = 0$ and $f(\cdot_1, \cdot_2) \in C^r$ for $r > 3$, then:

$$R_h(\phi^p) = A_{-2}(\phi). \tag{8.7}$$

Unless otherwise noted, a superscript p will henceforth denote a filter satisfying $\rho'(\pm\pi) = 0$. We note that the application of the filter is essential for the results in Equations (8.6) and (8.7) due to aliasing error. To see this, consider the following example adapted from [9]. Let $g(\alpha) = e^{2i\alpha}$ and define:

$$f(\alpha, \alpha') = \frac{1}{2\pi}\big(g(\alpha) - g(\alpha')\big)\cot\Big(\frac{\alpha - \alpha'}{2}\Big),\ f(\alpha, \alpha) = \frac{g_\alpha(\alpha)}{\pi}, \tag{8.8}$$

and let $\phi_i = e^{i\alpha_i(\frac{N}{2}-1)}$. Then from the Lemma 8.0.7 below, and using the fact that $e^{i\alpha_i(\frac{N}{2}+1)}$ is aliased to $e^{i\alpha_i(-\frac{N}{2}+1)}$, we have:

$$\begin{aligned} R_h(\phi_i) = \frac{e^{2i\alpha_i}}{2\pi} &\sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i)\ \text{odd}}}^{\frac{N}{2}} e^{i\alpha_j(\frac{N}{2}-1)} \cot\Big(\frac{\alpha_i - \alpha_j}{2}\Big)(2h) \\ &- \frac{1}{2\pi} \sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i)\ \text{odd}}}^{\frac{N}{2}} e^{i\alpha_j(-\frac{N}{2}+1)} \cot\Big(\frac{\alpha_i - \alpha_j}{2}\Big)(2h), \\ &= -i\big(e^{2i\alpha_i} e^{i\alpha_i(\frac{N}{2}-1)} + e^{i\alpha_i(-\frac{N}{2}+1)}\big), \\ &= -2ie^{i\alpha_i(-\frac{N}{2}+1)} = -2ig(\alpha_i)\phi_i = A_0(\phi_i). \end{aligned} \tag{8.9}$$

Remark 8.0.6. *If no filtering is applied, then it is easy to see that:*

$$R_h(\phi) = A_0(\phi). \tag{8.10}$$

Indeed we note that by the Schwartz inequality,

$$\|R_h(\phi)\|_{l^2} = \left(h \sum_{i=-\frac{N}{2}+1}^{\frac{N}{2}} \left| \sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i) \text{ odd}}}^{\frac{N}{2}} f(\alpha_i, \alpha_j)\phi_j(2h) \right|^2 \right)^{\frac{1}{2}}$$

$$\leq 4h\|\phi\|_{l^2} \sum_{i=-\frac{N}{2}+1}^{\frac{N}{2}} \left(h \sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i) \text{ odd}}}^{\frac{N}{2}} |f(\alpha_i, \alpha_j)|^2 \right)$$

$$\leq 4\|f\|_{l^2}\|\phi\|_{l^2}, \tag{8.11}$$

where

$$\|f\|_{l^2} = \left(h^2 \sum_{i=-\frac{N}{2}+1}^{\frac{N}{2}} \sum_{j=-\frac{N}{2}+1}^{\frac{N}{2}} |f(\alpha_i, \alpha_j)|^2 \right)^{\frac{1}{2}}, \tag{8.12}$$

which gives the result in Equation (8.10).

The Hilbert transform $\mathcal{H}(\omega)$ is the leading order part (i.e., least regular term) in velocity expression Equation (4.23). The discrete version of $\mathcal{H}(\omega)$ is:

$$\mathcal{H}_h(\omega_i) = \frac{1}{2\pi} \sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i) \text{ odd}}}^{\frac{N}{2}} \omega_j \cot\left(\frac{\alpha_i - \alpha_j}{2}\right)(2h). \tag{8.13}$$

This will be seen to play a crucial rule in the stability of our discretization. The continuous Hilbert transform satisfies:

$$\widehat{(\mathcal{H}f)}_k = -i\text{sgn}(k)\hat{f}_k, \tag{8.14}$$

$$\mathcal{H}(\mathcal{H}f(\alpha)) = -f(\alpha), \tag{8.15}$$

$$\mathcal{H}(f_\alpha)(\alpha) = (\mathcal{H}f)_\alpha(\alpha) \tag{8.16}$$

for a periodic function f. The following lemma from [9] shows that the discrete transform acts in the same way.

Lemma 8.0.7. *Assume that f satisfies $\hat{f}_0 = \hat{f}_{\frac{N}{2}} = 0$. The discrete Hilbert transform defined by (8.13) satisfies the following properties:*

$$\widehat{(\mathcal{H}_h f)}_k = -i\text{sgn}(k)\hat{f}_k, \tag{8.17}$$

$$\mathcal{H}_h(\mathcal{H}_h f_i) = -f_i, \tag{8.18}$$

$$\mathcal{H}_h(S_h f_i) = S_h(\mathcal{H}_h f_i) = \frac{1}{\pi}\sum_{(j-i)\text{ odd}} \frac{f_i - f_j}{(\alpha_i - \alpha_j)^2}(2h). \tag{8.19}$$

where $\sum_{(j-i)\text{ odd}}$ is defined in (8.21) below. The first equality above also implies $\|\mathcal{H}_h f\|_{l^2} = \|f\|_{l^2}$.

Proof. We transform the kernel in Equation (8.13) from a representation in the periodic domain to an equivalent representation in the infinite domain. This involves application of the formula [34],

$$\frac{1}{2}\cot(\frac{z}{2}) = \frac{1}{z} + \sum_{k=1}^{\infty} \frac{2z}{z^2 - (2k\pi)^2}, \tag{8.20}$$

from which it is easy to obtain (see [9] for details):

$$\frac{1}{2}\sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i)\text{ odd}}}^{\frac{N}{2}} f(\alpha_j)\cot\left(\frac{\alpha_i - \alpha_j}{2}\right)(2h), = \lim_{M\to\infty} \sum_{\substack{j=-M(N+\frac{1}{2})+1 \\ (j-i)\text{ odd}}}^{N(M+\frac{1}{2})} \frac{f(\alpha_j)}{\alpha_i - \alpha_j}(2h),$$
$$\equiv \sum_{(j-i)\text{ odd}} \frac{f(\alpha_j)}{\alpha_i - \alpha_j}(2h). \tag{8.21}$$

From Equations (8.13) and (8.21) with f_j in replace of $f(\alpha_j)$, it follows that:

$$\mathcal{H}_h(f_i) = \frac{1}{\pi}\sum_{(j-i)\text{ odd}} \frac{f_j}{\alpha_i - \alpha_j}(2h), \tag{8.22}$$

which is an equivalent form of the discrete Hilbert transform. This form is proven to satisfy properties (Equations (8.17)-(8.19)) in [9]. □

We will also need the following lemma on the commutator of the discrete Hilbert transform and a smooth function, from [9].

Theorem 8.0.8. *Let $g(\cdot) \in C^r$ for $r > 3$, and define the commutator*

$$\big[\mathcal{H}_h, g\big](\phi^p) = \mathcal{H}_h(g(\alpha_i)\phi^p) - g(\alpha_i)\mathcal{H}_h(\phi_i^p). \tag{8.23}$$

Then $\big[\mathcal{H}_h, g\big](\phi^p) \in A_{-1}(\phi^p)$. If in addition $\rho(x)$ satisfies $\rho'(\pm\pi) = 0$ and $g(\cdot) \in C^r$ with $r > 4$, then $\big[\mathcal{H}_h, g\big](\phi^p) \in A_{-2}(\phi^p)$.

Proof. Let:

$$f(\alpha, \alpha') = \frac{1}{2\pi}\big(g(\alpha) - g(\alpha')\big)\cot\left(\frac{\alpha - \alpha'}{2}\right) \in C^{r-1} \tag{8.24}$$

and apply Lemma 8.0.5. The result follows from noting that for this f,

$$R_h(\phi_i^p) = \mathcal{H}_h(g(\alpha_i)\phi^p) - g(\alpha_i)\mathcal{H}_h(\phi_i^p). \tag{8.25}$$

□

We will also need a lemma on the commutator of the filtering operator and a smooth function. The proof can be found in [12].

Lemma 8.0.9. *Let $f(\alpha_i) \in C^r$ for $r \geq 2$, and $\phi \in l^2$. Define:*

$$G_h^p(\phi_i) = \big(f(\alpha_i)\phi_i\big)^p - f(\alpha_i)\phi_i^p. \tag{8.26}$$

Then $G_h^p(\phi_i) = hA_0(\phi_i)$.

In our stability analysis, we will need an analogue of the product rule for discrete derivative operators, proven in [9].

Lemma 8.0.10. *Assume $f(\cdot) \in C^3$ and $w \in l^2$. Then we have:*

$$D_h(f(\alpha_i)w_i) = f(\alpha_i)D_h(w_i) + w_i^q f_\alpha(\alpha_i) + hA_0(w_i), \tag{8.27}$$

where $\hat{w}_k^q = \hat{w}_k q(kh)$ and $q(x) = \frac{\partial}{\partial x}(x\rho(x))$, and A_0 is a bounded operator.

We will apply the following lemmas to obtain expressions for the variation of velocities and other quantities in our problem. Define the error to be:

$$\dot{f}_i = f_i - f(\alpha_i). \tag{8.28}$$

Lemma 8.0.11. *Let* $\dot{f}_i, \dot{g}_i$ *and* $f(\alpha_i), g(\alpha_i)$ *be as defined in (8.28). Then* $\big(f_i g_i\big)^{\cdot} = \dot{f}_i g(\alpha_i) + f(\alpha_i)\dot{g}_i + \dot{f}_i\dot{g}_i$.

Proof.

$$\begin{aligned}
\big(f_i g_i\big)^{\cdot} &= f_i g_i - f(\alpha_i)g(\alpha_i) \\
&= f_i g(\alpha_i) - f(\alpha_i)g(\alpha_i) + f_i g_i - f_i g(\alpha_i) \\
&= (f_i - f(\alpha_i))g(\alpha_i) + f_i(g_i - g(\alpha_i)) \\
&= \dot{f}_i g(\alpha_i) + f_i \dot{g}_i \\
&= \dot{f}_i g(\alpha_i) + (f(\alpha_i) + \dot{f}_i)\dot{g}_i \\
&= \dot{f}_i g(\alpha_i) + f(\alpha_i)\dot{g}_i + \dot{f}_i\dot{g}_i. \qquad (8.29)
\end{aligned}$$

Note if $\dot{f}_i$ is $\mathrm{O}(h^{m_1})$, and if $\dot{g}_i$ has error $\mathrm{O}(h^{m_2})$, then $\big(\dot{fg}\big)_i$ is $\mathrm{O}(h^{\min\{m_1,m_2\}})$. □

The above lemma can be easily extended to product of three or more quantities. We also have:

Lemma 8.0.12.

$$\left(\frac{1}{f_i}\right)^{\cdot} = -\frac{\dot{f}_i}{f^2(\alpha_i)} + \frac{\dot{f}_i^2}{f^2(\alpha_i)\big(f(\alpha_i) + \dot{f}_i\big)}. \tag{8.30}$$

Proof.

$$\left(\frac{1}{f_i}\right)^{\cdot} = \frac{1}{f_i} - \frac{1}{f(\alpha_i)} = \frac{f(\alpha_i) - f_i}{f_i f(\alpha_i)} = -\frac{\dot{f}_i}{f(\alpha_i)\big(f(\alpha_i) + \dot{f}_i\big)}, \tag{8.31}$$

where in the last equality, we have eliminated f_i using $f_i = f(\alpha_i) + \dot{f}_i$. After decomposing the right hand side of (8.30) into a sum of linear and nonlinear parts in $\dot{f}_i$, we obtain the result (8.30). □

We will need the following results on $\dot{\sigma} = \sigma - s_\alpha$.

Lemma 8.0.13. *Let f be a smooth function and $\langle f(\cdot)\sigma\rangle_h = 0$. Then:*

$$S_h^{-1}\big(f(\cdot)\dot{\sigma}\big)_i = \dot{\sigma} S_h^{-1}\big(f(\cdot)\big)_i = A_{-s}(\dot{\sigma}_i), \tag{8.32}$$

where $A_{-s}(\dot{\sigma}_i)$ is here interpreted for the spatially independent $\dot{\sigma}$ as

$$A_{-s}(\dot{\sigma}_i) = \dot{\sigma} g(\alpha_i) \tag{8.33}$$

for some smooth function g.

Proof. The relation (Equation (8.32)) follows from the spatial independence of $\dot{\sigma}$. The second equality follows from the smoothness of f. □

Similarly we have:

Lemma 8.0.14. *Let f be a smooth function. Then:*

$$S_h\big(f(\cdot)\dot{\sigma}\big)_i = f_\alpha(\alpha_i)\dot{\sigma} = A_{-s}(\dot{\sigma}_i) + O(h^s), \tag{8.34}$$

and the same is true for D_h instead of S_h.

Proof. We have

$$S_h\big(f(\cdot)\dot{\sigma}\big)_i = \dot{\sigma} S_h f(\alpha_i) = \dot{\sigma} f_\alpha(\alpha_i) + \mathrm{O}(h^s), \tag{8.35}$$

and (8.34) immediately follows. □

We will make repeated use of the following result from [13]:

Lemma 8.0.15. *For $\dot{\theta}, \dot{\sigma}$ satisfying $\|\dot{\theta}\|_\infty \le h^3, \|\dot{\sigma}\|_\infty < h^3$, then:*

$$\big(\sigma e^{i\theta}\big)^{\dot{}}_i = i s_\alpha e^{i\theta(\alpha_i)}\dot{\theta}_i + e^{i\theta(\alpha_i)}\dot{\sigma}_i + A_{-3}(\dot{\theta}_i) = O(h^3). \tag{8.36}$$

Proof. We have:

$$\begin{aligned}\left(\sigma e^{i\theta}\right)^{\cdot}_i &= \sigma e^{i\theta_i} - s_\alpha e^{i\theta(\alpha_i)},\\ &= s_\alpha e^{i\theta(\alpha_i)}\left(e^{i\dot{\theta}_i} - 1\right) + \left(\sigma - s_\alpha\right)e^{i\theta(\alpha_i)}e^{i\dot{\theta}_i},\\ &= s_\alpha e^{i\theta(\alpha_i)}\left(i\dot{\theta}_i + r(\dot{\theta}_i)\right) + \dot{\sigma}_i e^{i\theta(\alpha_i)}\left(1 + i\dot{\theta}_i + r(\dot{\theta}_i)\right),\end{aligned} \tag{8.37}$$

where $\|r(\dot{\theta})\|_{l^2} \leq \|\dot{\theta}^2\|_{l^2} \leq h^3\|\dot{\theta}\|_{l^2}$. The first equality in Equation (8.36) follows by using $\|\dot{\sigma}\|_\infty \leq h^3$ and the above estimate on $\|r(\dot{\theta})\|_{l^2}$ to show that the nonlinear terms in the variation are $A_{-3}(\dot{\theta})$. The second equality in Equation (8.36) readily follows from Equation (8.37) and the bounds $\|\dot{\theta}\|_\infty \leq h^3$, $\|\dot{\sigma}\|_\infty < h^3$, and the above estimate on $\|r(\dot{\theta})\|_{l^2}$. □

Lemma 8.0.16. *Let ζ_i represent the discretized interface. Then:*

$$\dot{\zeta}_i = iS_h^{-1}\left(\sigma e^{i\theta(\cdot)}\dot{\theta}\right)_i + A_{-3}(\dot{\theta}_i) + A_{-s}(\dot{\sigma}) + \dot{\zeta}_c. \tag{8.38}$$

It will also be shown later that $\dot{\zeta}_c = O(h^{\frac{5}{2}})$.

Proof. Recall that

$$\zeta_i = S_h^{-1}\left(\sigma e^{i\theta} - \langle\sigma e^{i\theta}\rangle_h\right)_i + \zeta_c, \tag{8.39}$$

where $\zeta_c = \hat{\zeta}_0$ is the time dependent $k = 0$ Fourier mode of ζ_i. Taking the variation, we have:

$$\dot{\zeta}_i = S_h^{-1}\left((\sigma e^{i\theta})^{\cdot}_i - \langle(\sigma e^{i\theta})^{\cdot}\rangle_h\right) + \dot{\zeta}_c. \tag{8.40}$$

We now substitute the first equality in Equation (8.36) and use Lemma 8.0.19 below, which states that for $f \in C^s$ and an arbitrary variation $\dot{\phi}$, $\langle f(\cdot)\dot{\phi}\rangle_h = A_{-s}(\dot{\phi})$. Hence,

$$\begin{aligned}\dot{\zeta}_i = iS_h^{-1}&\left(\sigma e^{i\theta(\cdot)}\dot{\theta}\right)_i + S_h^{-1}\left(e^{i\theta(\cdot)}\dot{\sigma}\right)\\ &+ \dot{\zeta}_c + A_{-3}(\dot{\theta}) + A_{-s}(\dot{\sigma}).\end{aligned} \tag{8.41}$$

Finally, from Lemma 8.0.14, the second term on the right hand side of the above relation is $A_{-s}(\dot{\sigma})$, which proves the result. $\square$

Remark 8.0.17. *Evidentally, we also have from Equation (8.40):*

$$S_h\dot{\zeta}_i = \big((\sigma e^{i\theta})_i^{\cdot} - \langle(\sigma e^{i\theta})_i^{\cdot}\rangle_h\big), \tag{8.42}$$

and following the same reasoning as in the proof of Lemma 8.0.16:

$$\begin{aligned} S_h\dot{\zeta}_i &= is_\alpha e^{i\theta(\alpha_i)}\dot{\theta}_i + A_{-3}(\dot{\theta}_i) + A_{-s}(\dot{\sigma}) \\ &= A_0(\dot{\theta}_i) + A_{-s}(\dot{\sigma}). \end{aligned} \tag{8.43}$$

Since $\|\dot{\theta}\|_{l^2} \leq h^{\frac{7}{2}}, \|\dot{\sigma}\|_{l^2} < h^{\frac{7}{2}}$ and $\|\dot{\theta}\|_\infty \leq h^3, \|\dot{\sigma}\|_\infty < h^3$, we see from this analysis that $\|S_h\dot{\zeta}\|_{l^2} \leq h^{\frac{7}{2}}$ and $\|S_h\dot{\zeta}\|_\infty \leq h^3$.

In estimating the variations, we will make use of the discrete Parseval equality. First, recall that we may write the l^2 inner product as:

$$\big(f, g\big)_h = h \sum_{i=-\frac{N}{2}+1}^{\frac{N}{2}} \overline{f_i} g_i, \tag{8.44}$$

for $f, g \in l^2$. Then, we have:

Lemma 8.0.18. *(Discrete Parseval's equality). Let $f, g \in l^2$. Then:*

$$\big(f, g\big)_h = 2\pi \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} \overline{\hat{f}_k} \hat{g}_k. \tag{8.45}$$

In particular, when $g_i = f_i$:

$$\|f\|_{l^2}^2 = 2\pi \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} |\hat{f}_k|^2. \tag{8.46}$$

A simple consequence of Parseval's equality is that derivatives can be transformed to a smooth function, similar to integration by parts.

Lemma 8.0.19. *Let* $f(\cdot) \in C^{s+1}$ *and* $g \in l^2$*, then:*

$$\big(f(\cdot), S_h g\big)_h = -\big(S_h f(\cdot), g\big)_h \in A_{-s}(g). \tag{8.47}$$

The same result holds for the discrete average:

$$\langle f(\cdot) S_h g \rangle_h = -\langle g S_h f(\cdot) \rangle_h \in A_{-s}(g). \tag{8.48}$$

Thus, when considered as an operator Q *on* g*,*

$$Q(g) \equiv \langle f(\cdot) g \rangle_h \in A_{-(s+1)}(g). \tag{8.49}$$

Proof. By Parseval's equality:

$$\begin{aligned}\big(f(\cdot), S_h g\big)_h &= 2\pi \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} \overline{\hat{f}_k}(ik)\hat{g}_k \\ &= 2\pi \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} \overline{(-ik)\hat{f}_k}\hat{g}_k \\ &= -\big(S_h(f(\cdot)), g\big)_h.\end{aligned} \tag{8.50}$$

The result on discrete average follows from:

$$\langle f(\cdot) g \rangle_h = \frac{1}{2\pi}\big(\overline{f}, g\big)_h. \tag{8.51}$$

□

Note these results also hold for D_h. We will also make use of the fact that $S_h^{-1}(f(\cdot)\phi)_i$ is a smoothing operator on ϕ. The proof of this includes, as a by product, an 'integration by parts' formula for S_h^{-1}.

Lemma 8.0.20. *Let* $f \in C^3$*,* $\phi \in l^2$*, and assume* $f(\cdot)\phi_i$ *has zero mean, i.e.,* $\langle f(\cdot)\phi \rangle_h \equiv 0$*. Then:*

$$S_h^{-1}(f(\cdot) S_h \phi)_i = -S_h^{-1}(S_h f(\cdot)\phi)_i + f(\cdot)\phi_i + A_0(\phi_i), \tag{8.52}$$

and hence:

$$S_h^{-1}(f(\cdot)\phi)_i = A_{-1}(\phi_i). \tag{8.53}$$

The proof of Lemma 8.0.20 is technical and relegated to the appendix.

CHAPTER 9

ESTIMATES FOR THE VARIATION OF VELOCITIES

The discrete equation for velocity is given by Equation (4.12). We rewrite the equation as $u_i = U_{1,i} + U_{2,i} + U_{3,i} + U_{4,i}$, where:

$$U_{1,i} = \mathcal{H}_h\omega_i = -\frac{h}{\pi}\sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\ \text{odd}}}^{\frac{N}{2}} \omega_j^p\Big(2\text{Re}\Big(\frac{S_h\zeta_j}{\zeta_j-\tau_i}\Big)+\cot\Big(\frac{\alpha_i-\alpha_j}{2}\Big)\Big), \tag{9.1}$$

$$U_{2,i} = \frac{h}{\pi}\sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\ \text{odd}}}^{\frac{N}{2}} \frac{\overline{\omega}_j^p S_h\zeta_j}{\overline{\zeta_j}-\overline{\tau_i}}, \tag{9.2}$$

$$U_{3,i} = -\frac{h}{\pi}\sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\ \text{odd}}}^{\frac{N}{2}} \frac{\overline{\omega}_j^p(\zeta_j-\tau_i)\overline{S_h\zeta_j}}{(\overline{\zeta_j}-\overline{\tau_i})^2}, \tag{9.3}$$

$$U_{4,i} = (Q+iB)\tau_i - \frac{iG\tau_i}{2}, \tag{9.4}$$

for $i = -\frac{N}{2}+1,\cdots,\frac{N}{2}$. Note that $\mathcal{H}_h(\omega_i)$ has been substituted for the sum with cotangent kernel in Equation (4.12).

Variations of the $U_{l,i}, l = 1,2,\cdots,4$ are calculated using Lemmas 8.0.11 and 8.0.12. We represent these variations as the sum of linear and nonlinear quantities in the variation, so that:

$$\begin{aligned}\dot{U}_{1,i} = \mathcal{H}_h\dot{\omega}_i &- \frac{h}{\pi}\sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\ \text{odd}}}^{\frac{N}{2}} \dot{\omega}_j^p\Big(2\text{Re}\Big(\frac{S_h\zeta_h(\alpha_j)}{\zeta_h(\alpha_j)-\tau_h(\alpha_i)}\Big)+\cot\Big(\frac{\alpha_i-\alpha_j}{2}\Big)\Big)\\ &- \frac{h}{\pi}\sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\ \text{odd}}}^{\frac{N}{2}} \Big(\omega^p(\alpha_j)2\text{Re}\Big(\frac{S_h\dot{\zeta}_j}{\zeta_h(\alpha_j)-\tau_h(\alpha_i)} - \frac{S_h\zeta_h(\alpha_j)}{(\zeta_h(\alpha_j)-\tau_h(\alpha_i))^2}(\dot{\zeta}_j-\dot{\tau}_i)\Big)\Big)\\ &+ \dot{U}_{1,i}^{NL},\end{aligned} \tag{9.5}$$

where:

$$\dot{U}_{1,i}^{NL} = -\frac{h}{\pi} \sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i)\text{ odd}}}^{\frac{N}{2}} \left\{ \dot{\omega}_j^p \left(2\mathrm{Re}\Big(\frac{S_h \zeta_j}{\zeta_j - \tau_i} \Big)^{\cdot} \right) + \omega^p(\alpha_j) \left[2\mathrm{Re}\left(S_h \dot{\zeta}_j \Big(\frac{1}{\zeta_j - \tau_i} \Big)^{\cdot} \right) \right] \right.$$

$$\left. + \, \omega^p(\alpha_j) 2\mathrm{Re}\left(\frac{S_h \zeta_h(\alpha_j)\big(\dot{\zeta}_j - \dot{\tau}_i\big)^2}{[\zeta_h(\alpha_j) - \tau_h(\alpha_i)]^2 \big(\zeta_h(\alpha_j) - \tau_h(\alpha_i) + (\dot{\zeta})_j - (\dot{\tau})_i\big)} \right) \right\}. \qquad (9.6)$$

Note that the third term within brackets the above comes from the nonlinear term in the variation of $\left(\frac{1}{\zeta_j - \tau_i}\right)^{\cdot}$, via Equation (8.30). Similarly,

$$\dot{U}_{2,i} = \frac{h}{\pi} \sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i)\text{ odd}}}^{\frac{N}{2}} \left[\frac{\overline{\dot{\omega}_j^p} S_h \zeta_h(\alpha_j) + \overline{\omega^p}(\alpha_j) S_h \dot{\zeta}_j}{\overline{\zeta_h}(\alpha_j) - \overline{\tau_h}(\alpha_i)} - \big(\overline{\dot{\zeta}_j} - \overline{\dot{\tau}_i}\big) \frac{\overline{\omega_h}(\alpha_j) S_h \zeta_h(\alpha_j)}{[\overline{\zeta_h}(\alpha_j) - \overline{\tau_h}(\alpha_i)]^2} \right]$$

$$+ \, \dot{U}_{2,i}^{NL}, \qquad (9.7)$$

To compactly represent the nonlinear term, introduce the notation:

$$[f_i, g_i, h_i]^{\cdot} = \dot{f}_i \dot{g}_i h(\alpha_i) + \dot{f}_i g(\alpha_i) \dot{h}_i + f(\alpha_i) \dot{g}_i \dot{h}_i, \qquad (9.8)$$

which gives the nonlinear terms in the variation of the product fgh. A similar notation is used for the nonlinear terms in the variation of a product with four or more functions. Then,

$$\dot{U}_{2,i}^{NL} = \frac{h}{\pi} \sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i)\text{ odd}}}^{\frac{N}{2}} \left\{ \left[\overline{\omega}_j^p, S_h \zeta_j, \frac{1}{\overline{\zeta_j} - \overline{\tau_i}} \right]^{\cdot} \right.$$

$$\left. + \, \frac{\overline{\omega_h}(\alpha_j) S_h \zeta_h(\alpha_j) \big(\overline{\dot{\zeta}_j} - \overline{\dot{\tau}_i}\big)^2}{[\overline{\zeta_h}(\alpha_j) - \overline{\tau_h}(\alpha_i)]^2 \big(\overline{\zeta_h}(\alpha_j) - \overline{\tau_h}(\alpha_i) + \overline{\dot{\zeta}_j^p} - \overline{\dot{\tau}_i^p}\big)} \right\}, \qquad (9.9)$$

where for example in $\left[\overline{\omega}_j^p, S_h\zeta_j, \frac{1}{\overline{\zeta_j}-\overline{\tau_i}}\right]^{\cdot}$, if $g_j = S_h\zeta_j$, then $g(\alpha_j) = S_h\zeta_h(\alpha_j)$. Continuing,

$$\begin{aligned}\dot{U}_{3,i} = -\frac{h}{\pi} \sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\text{ odd}}}^{\frac{N}{2}} &\Bigg[\Big(\dot{\overline{\omega}}_j^p\big[\zeta_h(\alpha_j) - \tau_h(\alpha_i)\big]\overline{S_h\zeta_h}(\alpha_j) + \overline{\omega^p}(\alpha_j)\big[\dot{\zeta}_j - \dot{\tau}_i\big]\overline{S_h\zeta_h}(\alpha_j)\\
&+ \overline{\omega^p}(\alpha_j)\big[\zeta_h(\alpha_j) - \tau_h(\alpha_i)\big]\overline{S_h\dot{\zeta}_j}\Big)\left(\frac{1}{\overline{\zeta_h}(\alpha_j) - \overline{\tau_h}(\alpha_i)}\right)^2\\
&- \frac{2\overline{\omega^p}(\alpha_j)\big[\zeta_h(\alpha_j) - \tau_h(\alpha_i)\big]\overline{S_h\zeta_h}(\alpha_j)\big[\dot{\overline{\zeta_j}} - \dot{\overline{\tau_i}}\big]}{\big[\overline{\zeta_h}(\alpha_j) - \overline{\tau_h}(\alpha_i)\big]^3}\Bigg]\\
&+ \dot{U}_{3,i}^{NL},\end{aligned} \tag{9.10}$$

where,

$$\begin{aligned}\dot{U}_{3,i}^{NL} = -\frac{h}{\pi} \sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\text{ odd}}}^{\frac{N}{2}} &\Bigg\{\left[\overline{\omega_j^p}, \zeta_j - \tau_i, \overline{S_h\zeta_j}, \frac{1}{\overline{\zeta_j} - \overline{\tau_i}}, \frac{1}{\overline{\zeta_j} - \overline{\tau_i}}\right]^{\cdot}\\
&+ \frac{\overline{\omega^p}(\alpha_j)\big[\zeta_h(\alpha_j) - \tau_h(\alpha_i)\big]\overline{S_h\zeta_h}(\alpha_j)\big[\dot{\overline{\zeta_j}} - \dot{\overline{\tau_i}}\big]^2}{[\overline{\zeta_h}(\alpha_j) - \overline{\tau_h}(\alpha_i)]^2\big(\overline{\zeta_h}(\alpha_j) - \overline{\tau_h}(\alpha_i) + \dot{\overline{\zeta_j}} - \dot{\overline{\tau_i}}\big)}\Bigg\}.\end{aligned} \tag{9.11}$$

Finally,

$$\dot{U}_{4,i} = (Q + iB)\dot{\overline{\tau_i}} - \frac{iG\dot{\tau}_i}{2}. \tag{9.12}$$

In the next section, we compute the leading order contribution to the variation in the velocity. This computation uses the following integral estimates.

Lemma 9.0.1. *Let $\dot{q} \in l^2$ be a variation of some quantity, and let:*

$$I_h\dot{q}_i = \frac{h}{\pi} \sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\text{ odd}}}^{\frac{N}{2}} \frac{f(\alpha_j)\dot{q}_j}{\zeta(\alpha_j) - \zeta(\alpha_i)}, \tag{9.13}$$

with $f(\alpha)$ and $\zeta(\alpha)$ smooth, and $\zeta_\alpha(\alpha) \neq 0$. Define:

$$K_{1h}[f,\zeta](\dot{q}_i) = \frac{h}{\pi} \sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i)\ \mathrm{odd}}}^{\frac{N}{2}} \dot{q}_j \Big[\frac{f(\alpha_j)}{\zeta(\alpha_j)-\zeta(\alpha_i)} - \frac{f(\alpha_i)}{2\zeta_\alpha(\alpha_i)} \cot\Big(\frac{\alpha_j-\alpha_i}{2}\Big)\Big]. \tag{9.14}$$

Then:

$$I_h \dot{q}_i = -\frac{f(\alpha_i)}{2\zeta_\alpha(\alpha_i)} \mathcal{H}_h \dot{q}_i + K_{1h}[f,\zeta](\dot{q}_i), \tag{9.15}$$

and $K_{1h}[f,\zeta](\dot{q}_i^p) = A_{-2}(\dot{q}_i^p)$, when filtering is applied.

Proof. The decomposition in (9.15) follows from adding and substracting $-\frac{f(\alpha_i)}{2\zeta_\alpha(\alpha_i)}\mathcal{H}_h q_i$. The fact that K_{1h} is a smoothing operator on $\dot{q}^p$ then follows by noting that the kernel within brackets in K_{1h} is smooth, and applying Lemma 8.0.5. □

Lemma 9.0.2. *Under the same assumptions as in Lemma 8.0.18, let:*

$$J_h \dot{\zeta}_i = \frac{h}{\pi} \sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i)\ \mathrm{odd}}}^{\frac{N}{2}} \frac{f(\alpha_j)\big(\dot{\zeta}_j - \dot{\zeta}_i\big)}{\big[\zeta(\alpha_j)-\zeta(\alpha_i)\big]^2}, \tag{9.16}$$

and define:

$$K_{2h}[f,\zeta](\dot{\zeta}_i) = \frac{h}{\pi} \sum_{\substack{j=-\frac{N}{2}+1 \\ (j-i)\ \mathrm{odd}}}^{\frac{N}{2}} \big(\dot{\zeta}_j - \dot{\zeta}_i\big) \Bigg[\frac{f(\alpha_j)}{\big[\zeta(\alpha_j)-\zeta(\alpha_i)\big]^2} - \frac{f(\alpha_i)}{4\zeta_\alpha^2(\alpha_i)\sin^2\big(\frac{\alpha_j-\alpha_i}{2}\big)}$$
$$- \frac{f_\alpha(\alpha_i) - \frac{\zeta_{\alpha\alpha}(\alpha_i)}{\zeta_\alpha(\alpha_i)} f_\alpha(\alpha_i)}{2\zeta_\alpha^2(\alpha_i)} \cot\Big(\frac{\alpha_j-\alpha_i}{2}\Big)\Bigg]. \tag{9.17}$$

Then:

$$J_h \dot{\zeta}_i = -\frac{f(\alpha_i)}{2\zeta_\alpha^2(\alpha_i)} \mathcal{H}_h(S_h \dot{\zeta}_i) - \frac{f_\alpha(\alpha_i) - \frac{\zeta_{\alpha\alpha}(\alpha_i)}{\zeta_\alpha(\alpha_i)} f_\alpha(\alpha_i)}{2\zeta_\alpha^2(\alpha_i)} \mathcal{H}_h \dot{\zeta}_i$$
$$+ K_{2h}[f,\zeta](\dot{\zeta}_i), \tag{9.18}$$

and:

$$K_{2h}[f,\zeta](\dot{\zeta}_i^p) = A_{-2}(\dot{\zeta}_i^p). \tag{9.19}$$

Proof. Write:

$$\frac{h}{\pi}\sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\text{ odd}}}^{\frac{N}{2}}\frac{f(\alpha_j)\big(\dot\zeta_j-\dot\zeta_i\big)}{\big[\zeta(\alpha_j)-\zeta(\alpha_i)\big]^2}=\frac{h}{\pi}\left[\frac{f(\alpha_i)}{4\zeta_\alpha^2(\alpha_i)}\sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\text{ odd}}}^{\frac{N}{2}}\frac{\dot\zeta_j-\dot\zeta_i}{\sin^2\left(\frac{\alpha_j-\alpha_i}{2}\right)}\right.$$
$$\left.+\frac{f_\alpha(\alpha_i)-\frac{\zeta_{\alpha\alpha}(\alpha_i)}{\zeta_\alpha(\alpha_i)}f_\alpha(\alpha_i)}{2\zeta_\alpha^2(\alpha_i)}\sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\text{ odd}}}^{\frac{N}{2}}\big(\dot\zeta_j-\dot\zeta_i\big)\cot\left(\frac{\alpha_j-\alpha_i}{2}\right)\right]$$
$$+K_2[f,\zeta](\dot\zeta^p) \tag{9.20}$$

by adding and subtracting $\frac{h}{\pi}$ times the quantities in brackets. Next use the identity:

$$\frac{1}{\sin^2\frac{z}{2}}=4\sum_{n=-\infty}^{\infty}\frac{1}{(z-2n\pi)^2} \tag{9.21}$$

to write:

$$\sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\text{ odd}}}^{\frac{N}{2}}\frac{\dot\zeta_j-\dot\zeta_i}{\sin^2\left(\frac{\alpha_j-\alpha_i}{2}\right)}=4\lim_{M\to\infty}\sum_{\substack{j=-N(M+\frac{1}{2})+1\\(j-i)\text{ odd}}}^{N(M+\frac{1}{2})}\frac{\dot\zeta_j-\dot\zeta_i}{\big(\alpha_j-\alpha_i\big)^2}, \tag{9.22}$$

where we have used the periodicity of $\dot\zeta_j$. Henceforth, we will use the notation $\sum_{(j-i)\text{ odd}}=\lim_{M\to\infty}\sum_{\substack{j=-N(M+\frac{1}{2})+1\\(j-i)\text{ odd}}}^{N(M+\frac{1}{2})}$. Substitute (9.22) for the first sum within the brackets in (9.20), and note that:

$$\mathcal{H}_h(S_h\dot\zeta_i)=\frac{h}{\pi}\sum_{(j-i)\text{ odd}}\frac{\dot\zeta_i-\dot\zeta_j}{(\alpha_i-\alpha_j)^2}, \tag{9.23}$$

and:

$$\mathcal{H}_h\dot\zeta_i=-\frac{h}{\pi}\sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\text{ odd}}}^{\frac{N}{2}}\big(\dot\zeta_j-\dot\zeta_i\big)\cot\left(\frac{\alpha_j-\alpha_i}{2}\right), \tag{9.24}$$

to obtain Equation (9.18). In Equation (9.24) we have used the identity

$$\sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\text{ odd}}}^{\frac{N}{2}} f_i \cot\left(\frac{\alpha_j-\alpha_i}{2}\right)=0 \tag{9.25}$$

which holds for a generic f. Finally, Equation (9.19) follows from the observation that the quantity within brackets in the definition of K_{2h} in Equation (9.17), namely,

$$\begin{aligned} g(\alpha,\alpha') = {} & \frac{f(\alpha')}{[\zeta(\alpha')-\zeta(\alpha)]^2} - \frac{f(\alpha)}{4\zeta_\alpha^2(\alpha)\sin^2\left(\frac{\alpha'-\alpha}{2}\right)} \\ & - \frac{f_\alpha(\alpha)-\frac{\zeta_{\alpha\alpha}(\alpha)}{\zeta_\alpha(\alpha)}f_\alpha(\alpha)}{2\zeta_\alpha^2(\alpha)}\cot\left(\frac{\alpha'-\alpha}{2}\right) \end{aligned} \tag{9.26}$$

is a smooth function of α and α'. □

Remark 9.0.3. *If filtering is not applied, then it is easy to see that* $K_{1h}[\cdot,\cdot]\dot{q}=A_0(\dot{q})$ *and* $K_{2h}[\cdot,\cdot]\dot{\zeta}=A_0(\dot{\zeta})$. *Indeed, this is a consequence of the remark following Lemma 8.0.5.*

The following lemmas are derived similarly and are presented without proof.

Lemma 9.0.4. *Under the same assumptions as Lemma 8.0.18, let:*

$$L_h\dot{q}_i=\frac{h}{\pi}\sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\text{ odd}}}^{\frac{N}{2}}\frac{f(\alpha_j)\big(\zeta(\alpha_j)-\zeta(\alpha_i)\big)\dot{q}_j}{\left[\overline{\zeta(\alpha_j)}-\overline{\zeta(\alpha_i)}\right]^2}, \tag{9.27}$$

and define:

$$K_{3h}[f,\zeta](\dot{q}_i)=\frac{h}{\pi}\sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\text{ odd}}}^{\frac{N}{2}}\dot{q}_j\left[\frac{\big(\zeta(\alpha_j)-\zeta(\alpha_i)\big)f(\alpha_j)}{\left[\overline{\zeta(\alpha_j)}-\overline{\zeta(\alpha_i)}\right]^2}-\frac{f(\alpha_i)\zeta_\alpha(\alpha_i)}{2\overline{\zeta^2(\alpha_i)}}\cot\left(\frac{\alpha_i-\alpha_j}{2}\right)\right]. \tag{9.28}$$

Then:

$$L_h\dot{q}_i=-\frac{f(\alpha_i)\zeta_\alpha(\alpha_i)}{2\overline{\zeta^2(\alpha_i)}}\mathcal{H}_h\dot{q}_i+K_{3h}[f,\zeta](\dot{q}_i), \tag{9.29}$$

and $K_{3h}[f,\zeta](\dot{q}_i^p) = A_{-2}(\dot{q}_i)$.

Lemma 9.0.5. *Under the same assumption as Lemma 8.0.18, let:*

$$M_h\overline{\dot{\zeta}} = \frac{h}{\pi}\sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\text{ odd}}}^{\frac{N}{2}} \frac{f(\alpha_j)\big(\zeta(\alpha_j)-\zeta(\alpha_i)\big)\big(\overline{\dot{\zeta}_j}-\overline{\dot{\zeta}_i}\big)}{\big[\overline{\zeta(\alpha_j)}-\overline{\zeta(\alpha_i)}\big]^3}, \tag{9.30}$$

and define:

$$K_{4h}[f,\zeta](\overline{\dot{\zeta}_j}) = \frac{h}{\pi}\sum_{\substack{j=-\frac{N}{2}+1\\(j-i)\text{ odd}}}^{\frac{N}{2}} \big(\overline{\dot{\zeta}_j}-\overline{\dot{\zeta}_i}\big)\Bigg[\frac{\big(\zeta(\alpha_j)-\zeta(\alpha_i)\big)f(\alpha_j)}{\big[\overline{\zeta(\alpha_j)}-\overline{\zeta(\alpha_i)}\big]^2} - \frac{f(\alpha_i)\zeta_\alpha(\alpha_i)}{4\overline{\zeta_\alpha^3(\alpha_j)}\sin^2\left(\frac{\alpha_j-\alpha_i}{2}\right)} + \frac{p(\alpha_i)}{2\overline{\zeta_\alpha^3(\alpha_i)}}\cot\left(\frac{\alpha_j-\alpha_i}{2}\right)\Bigg], \tag{9.31}$$

where:

$$p(\alpha_i) = \frac{\zeta_\alpha(\alpha_i)f(\alpha_i)}{2}\left(\frac{\zeta_{\alpha\alpha}(\alpha_i)}{\zeta_\alpha(\alpha_i)} - \frac{3\overline{\zeta_{\alpha\alpha}(\alpha_i)}}{\overline{\zeta_\alpha(\alpha_i)}}\right) + \zeta_\alpha(\alpha_i)f_\alpha(\alpha_i). \tag{9.32}$$

Then:

$$M_h\overline{\dot{\zeta}_i} = -\frac{f_\alpha(\alpha_i)\zeta_\alpha(\alpha_i)}{2\overline{\zeta_\alpha^3(\alpha_i)}}\mathcal{H}_h(\overline{S_h\dot{\zeta}_i}) - \frac{p(\alpha_i)}{2\overline{\zeta_\alpha^3(\alpha_i)}}\mathcal{H}_h\overline{\dot{\zeta}_i} + K_{4h}[f,\zeta](\overline{\dot{\zeta}_i}), \tag{9.33}$$

and $K_{4h}[f,\zeta](\overline{\dot{\zeta}_i^p}) = A_{-2}(\dot{\zeta}_i^p)$.

9.1 Leading Order Velocity Variations

We identify the most singular part in the variation $\dot{u}_i$ of the complex velocity. First, note that in Equations (9.5)-(9.7), we can replace ζ_h with ζ and $S_h\zeta_h$ with ζ_α, incurring by consistency an $O(h^s)$ error. (Recall that the expression $O(h^s)$ is used to denote a generic high-order discretization error). Now, consider $\dot{U}_1$ in Equation (9.5). We denote first sum in Equation (9.5) by $K_{0h}(\dot{\omega}_i^p)$, and apply Lemmas 9.0.1 and 9.0.2 to find,

$$
\begin{aligned}
\dot{U}_{1,i} &= \mathcal{H}_h(\dot{\omega}_i) - K_{0h}(\dot{\omega}_i^p) - K_{1h}[\omega^p,\zeta](S_h\dot{\zeta}_i) - K_{1h}[\omega^p,\overline{\zeta}](\overline{S_h\dot{\zeta}_i}) \\
&\quad - \omega_\alpha^p(\alpha_i)\Big(\frac{\mathcal{H}_h\dot{\zeta}_i}{2\zeta_\alpha(\alpha_i)} + \text{c.c.}\Big) + K_{2h}[\omega\zeta_\alpha,\zeta](\dot{\zeta}_i) + K_{2h}[\omega\overline{\zeta_\alpha},\overline{\zeta}](\overline{\dot{\zeta}_i}) \\
&\quad + \dot{U}_{1,i}^{NL} + \mathrm{O}(h^s), \qquad (9.34)
\end{aligned}
$$

where c.c. denote the complex conjugate of the previous term. The leading order contribution to $\dot{U}_{2,i}$ in Equation (9.7) is determined from Lemmas 9.0.1 and 9.0.2 as

$$
\begin{aligned}
\dot{U}_{2,i} &= -\frac{1}{2}\frac{\zeta_\alpha(\alpha_i)}{\overline{\zeta_\alpha}(\alpha_i)}\mathcal{H}_h\overline{\dot{\omega}_i^p} + K_{1h}[\zeta_\alpha,\overline{\zeta}](\overline{\dot{\omega}_i^p}) - \frac{\overline{\omega^p}(\alpha_i)}{2\overline{\zeta_\alpha}(\alpha_i)}\mathcal{H}_h(S_h\dot{\zeta}_i) + K_{1h}[\overline{\omega^p},\overline{\zeta}](S_h\dot{\zeta}_i) \\
&\quad + \frac{\overline{\omega^p}(\alpha_i)\zeta_\alpha(\alpha_i)}{2\overline{\zeta}_\alpha^2(\alpha_i)}\mathcal{H}_h(\overline{S_h\dot{\zeta}_i}) + \frac{1}{2\overline{\zeta}_\alpha^2(\alpha_i)}\big((\overline{\omega}^p\zeta_\alpha)_\alpha(\alpha_i) - \overline{\omega}^p(\alpha_i)\zeta_\alpha(\alpha_i)\overline{\zeta_{\alpha\alpha}}(\alpha_i)\big)\mathcal{H}_h(\overline{\dot{\zeta}_i}) \\
&\quad - K_{2h}[\overline{\omega}^p\zeta_\alpha,\overline{\zeta}](\overline{\dot{\zeta}_i}) + \dot{U}_{2,i}^{NL} + \mathrm{O}(h^s), \qquad (9.35)
\end{aligned}
$$

Similarly, we find from Equation (9.11) and Lemmas 9.0.2, 9.0.4 and 9.0.5 that

$$
\begin{aligned}
\dot{U}_{3,i} &= \frac{\zeta_\alpha(\alpha_i)}{2\overline{\zeta_\alpha}(\alpha_i)}\mathcal{H}_h\overline{\dot{\omega}_i^p} - K_{3h}[\overline{\zeta_\alpha},\zeta](\overline{\dot{\omega}_i^p}) + \frac{\overline{\omega^p}(\alpha_i)}{2\overline{\zeta_\alpha}(\alpha_i)}\mathcal{H}_h(S_h\dot{\zeta}_i) + \frac{\overline{\omega^p}(\alpha_i)}{2\overline{\zeta_\alpha}(\alpha_i)}\mathcal{H}_h\dot{\zeta}_i \\
&\quad - K_{2h}[\overline{\omega^p\zeta_\alpha},\overline{\zeta}](\dot{\zeta}_i) - \frac{\overline{\omega^p}(\alpha_i)\zeta_\alpha(\alpha_i)}{2\overline{\zeta}_\alpha^2(\alpha_i)}\mathcal{H}_h(\overline{S_h\dot{\zeta}_i}) - K_{3h}[\overline{\omega^p},\zeta](\overline{S_h\dot{\zeta}_i}) - \frac{p(\alpha_i)}{2\overline{\zeta}_\alpha^3(\alpha_i)}\mathcal{H}_h(\overline{\dot{\zeta}_i}) \\
&\quad + K_{4h}[2\overline{\omega^p\zeta_\alpha},\zeta](\overline{\dot{\zeta}_i}) + \dot{U}_{3,i}^{NL} + \mathrm{O}(h^s), \qquad (9.36)
\end{aligned}
$$

where:

$$
p(\alpha_i) = \overline{\omega}^p(\alpha_i)\big(\zeta_{\alpha\alpha}(\alpha_i)\overline{\zeta_\alpha}(\alpha_i) - 3\overline{\zeta_{\alpha\alpha}(\alpha_i)}\zeta_\alpha(\alpha_i)\big) + 2\zeta_\alpha(\alpha_i)(\overline{\omega\zeta_\alpha})_\alpha(\alpha_i). \qquad (9.37)
$$

Finally, $\dot{U}_{4,i}$ is easily seen to consist only of low order terms, i.e., involving smoothing operators. A more precise statement is given in the summary below.

9.2 Summary of Velocity Variation

The leading order contribution to the velocity variation is the sum of the contributions from $\dot{U}_l$ for $l = 1, \cdots, 4$. We anticipate the leading order contribution will come from

$\mathcal{H}_h\dot{\omega}_i$ in Equation (9.34) (the equation for $\dot{\omega}$ is derived and analyzed below). The leading order $\mathcal{H}_h\overline{\dot{\omega}_i^p}$ term in the sum of $\dot{U}_{2,i} + \dot{U}_{3,i}$ cancels out. This is related to the fact that the sum of the variation $\dot{U}_{2,i} + \dot{U}_{3,i}$ comes from the discretization of the integral

$$\int_\gamma \omega(\zeta, t) d\frac{\zeta - \tau}{\bar{\zeta} - \bar{\tau}}, \tag{9.38}$$

for which the kernel is smooth, i.e., the integrand is a smoothing operator on ω. Surprisingly, the next order terms in $\dot{U}_{2,i} + \dot{U}_{3,i}$ containing $\mathcal{H}_h S_h \dot{\zeta}_i$ and its conjugate, also cancel out. This is expected to have important consequences in the stability of the discrete equations in the drop problem, i.e., with $\mathcal{S}$ = constant and $\kappa_B = 0$; although this is beyond scope of current thesis.

To identify lower order terms in the velocity variation, we first use the Remark 8.0.17 to see that $S_h\dot{\zeta}_i = A_0(\dot{\theta}_i) + A_{-s}(\dot{\sigma}_i)$. Therefore, applying Remark 8.0.6, we have:

$$K_{\cdot h}[\cdot, \cdot](S_h\dot{\zeta}) = A_0(\dot{\theta}_i) + A_{-s}(\dot{\sigma}). \tag{9.39}$$

and similarly

$$K_{\cdot h}[\cdot, \cdot](\dot{\zeta}) = A_0(\dot{\theta}_i) + A_{-s}(\dot{\sigma}). \tag{9.40}$$

Lemma 8.0.5 implies that:

$$K_{1h}[\cdot, \cdot](\dot{\omega}^p) = A_{-2}(\dot{\omega}^p), \tag{9.41}$$

and

$$K_{2h}[\cdot, \cdot](\dot{\omega}^p) = A_{-2}(\dot{\omega}^p). \tag{9.42}$$

We also need to estimate $\dot{U}_4$ defined in Equation (9.12). From Lemma 8.0.16, we immediately see that:

$$\dot{U}_{4,i} = A_{-1}(\dot{\theta}_i) + A_{-s}(\dot{\sigma}) + \mathrm{O}(\dot{\zeta}_c). \tag{9.43}$$

Note that U_4 is the only velocity term in which $\zeta_c(t)$ appear. The other terms in our velocity decomposition, $U_1, \cdots, U_3$ depend only on the difference $\zeta_j - \tau_i$, for which ζ_c cancels out. In the appendix, we show that the nonlinear term satisfies

$$\dot{u}_i^{NL} = \sum_{n=1}^{4} \dot{U}_{n,i}^{NL} = A_0(\dot{\theta}) + A_{-s}(\dot{\sigma}) + \mathrm{O}(h^s). \tag{9.44}$$

Putting all the above facts together, we find from Equations (9.12),(9.34),(9.35),(9.36), and (9.43) that

$$\dot{u}_i = \sum_{l=1}^{4} \dot{U}_{l,i} = \mathcal{H}_h \dot{\omega}_i + A_{-2}(\dot{\omega}_i^p) + A_0(\dot{\theta}_i) + A_{-s}(\dot{\sigma}_i) + \mathrm{O}(|\dot{\zeta}_c|) + \mathrm{O}(h^s), \tag{9.45}$$

which is the main result of this section. Estimates on $\dot{\omega}$, which are combined with (9.45) to give $\dot{u}_i$ in terms of $\dot{\theta}$, $\dot{\sigma}$ and $\dot{\alpha_0}$ are provided in Section 9.3 below.

9.3 Tangential And Normal Velocity Variations

The discrete normal velocity is given by:

$$(u_n)_i = \mathrm{Re}\big\{u_i \overline{n_i}\big\} = \mathrm{Im}\big\{u_i e^{-i\theta_i}\big\}, \tag{9.46}$$

using $n_i = ie^{i\theta_i}$. We need the variation $\dot{u_n}_i$. From Equation (4.20), this is:

$$\begin{aligned}(\dot{u_n})_i = \frac{\kappa_B}{4s_\alpha^2}\mathcal{H}_h(S_h^2\dot{\theta}_i) + \frac{\kappa_B}{4}\Big(\frac{1}{2\sigma^2}\Big)^{\cdot}\mathcal{H}_h(\theta_{\alpha\alpha}(\alpha_i)) + \mathrm{Im}\big\{ - \big[\mathcal{H}, e^{-i\theta(\alpha_i)}\big](\dot{\omega}_i^p) \\ -\big[\mathcal{H}_h, (e^{-i\theta})^{\cdot}_i\big](\omega^p(\alpha_i)) + (\dot{u_R})_i e^{-i\theta(\alpha_i)} + u_R(\alpha_i)(e^{-i\theta})^{\cdot}_i\big\} + (\dot{u_n})_i^{NL} + \mathrm{O}(h^s),\end{aligned} \tag{9.47}$$

where $(\dot{u_n})_i^{NL}$ represents the nonlinear terms. It is straight forward to estimate each of the terms in Equation (9.47). Clearly,

$$\frac{\kappa_B}{4}\left(\frac{1}{\sigma^2}\right)^{\cdot}\mathcal{H}_h(\theta_{\alpha\alpha}(\alpha_i)) = A_{-s}(\dot{\sigma}_i), \tag{9.48}$$

(see e.g., Lemma 8.0.14). By Theorem 8.0.8,

$$\left[\mathcal{H}, e^{-i\theta(\alpha_i)}\right](\dot{\omega}_i^p) = A_{-2}(\omega_i^p). \tag{9.49}$$

It is also easy to see by following the same steps as the proof to Lemma 8.0.15 that

$$(e^{-i\theta})_i^{\cdot} = -ie^{-i\theta(\alpha_i)}\dot{\theta}_i + A_{-3}(\dot{\theta}_i), = \mathrm{O}(h^3), \tag{9.50}$$

and the first equality combined with Remark 8.0.6 show that

$$\left[\mathcal{H}_h, (e^{-i\theta})_i^{\cdot}\right](\omega^p(\alpha_i)) = A_0(\dot{\theta}). \tag{9.51}$$

Indeed, we can write

$$\begin{aligned}\left[\mathcal{H}_h, (e^{-i\theta})_i^{\cdot}\right](\omega^p(\alpha_i)) &= \mathcal{H}_h\big((e^{-i\theta})_i^{\cdot}(\omega^p(\alpha_i))\big) - \omega^p(\alpha_i)\mathcal{H}_h\big((e^{i\theta})_i^{\cdot}\big)\\ &+\omega^p(\alpha_i)\mathcal{H}_h\big((e^{i\theta})_i^{\cdot}\big) - (e^{i\theta})_i^{\cdot}\mathcal{H}_h(\omega^p(\alpha_i)),\end{aligned} \tag{9.52}$$

and note that the first two terms combine to form an integral operator with a smooth kernel on the (unfiltered) $(e^{i\theta})_i^{\cdot}$, and similar for the latter two terms. Remark 8.0.6 then implies (9.51). Furthermore, it is easy to see from Equation (4.16) that

$$(\dot{u_R})_i = A_{-2}(\dot{\omega}^p) + A_0(\dot{\theta}) + A_{-s}(\dot{\sigma}) + \mathrm{O}(\dot{\zeta}_c) + \mathrm{O}(h^s). \tag{9.53}$$

Finally, it is straightforward to show using the second equality in (9.50) and the previous estimate that

$$\|\dot{u_n}^{NL}\|_{l^2} = h^3\big(A_{-2}(\dot{\omega^p}) + A_0(\dot{\theta}) + A_{-s}(\dot{\sigma}) + \mathrm{O}(\dot{\zeta}_c) + \mathrm{O}(h^s)\big), \tag{9.54}$$

which we write as

$$(\dot{u_n})_i^{NL} = A_{-5}(\dot{\omega^p}) + A_{-3}(\dot{\theta}) + A_{-s}(\dot{\sigma}) + \mathrm{O}(h^3\dot{\zeta}_c) + \mathrm{O}(h^s). \tag{9.55}$$

Therefore, we have shown that

$$(\dot{u_n})_i = \frac{\kappa_B}{4s_\alpha^2}\mathcal{H}_h(S_h^2\dot{\theta}_i) + A_{-2}(\dot{\omega_i^p}) + A_0(\dot{\theta}_i) + A_{-s}(\dot{\sigma}) + \mathrm{O}(\dot{\zeta}_c) + \mathrm{O}(h^s). \tag{9.56}$$

We will also need the variation in the tangential velocity $\dot{u}_s$, since this appears in the evolution equation for $\dot{\alpha}_0$. We leave it to the reader to show, using the same arguments as for $(\dot{u_n})_i$, that:

$$\begin{aligned}(\dot{u_s})_i = &-\frac{\chi}{2}\mathcal{H}_h\big(\dot{\mathcal{S}}_i\big) + A_{-2}(\dot{\omega_i^p}) + A_0(\dot{\theta}_i) + A_{-s}(\dot{\sigma}) \\ &+ \mathrm{O}(\dot{\zeta}_c) + \mathrm{O}(h^s).\end{aligned} \tag{9.57}$$

Expressions for $\dot{\mathcal{S}}_i$ and $\dot{\omega}_i$ are given in Equations (9.62) and (9.74) below. These imply $\dot{\mathcal{S}}$ in Equation (9.57) can be replaced by $-\tilde{f}(\alpha_i)D_h\alpha_0 + A_{-1}(\dot{\alpha_0})$, where $\tilde{f}(\alpha)$ is defined in Equation (9.63) and $A_{-2}(\dot{\omega}^p)$ in Equations (9.56) and (9.74) replaced by $A_{-1}(\dot{\alpha_0})$.

Summarizing, we have shown that

$$(\dot{u_n})_i = \frac{\kappa_B}{4s_\alpha^2}\mathcal{H}_h(S_h^2\dot{\theta}_i) + A_0(\dot{\theta}) + A_{-s}(\dot{\sigma}) + A_{-1}(\dot{\alpha_0}) + \mathrm{O}(\dot{\zeta}_c) + \mathrm{O}(h^s), \tag{9.58}$$

$$\begin{aligned}(\dot{u_s})_i = &\frac{\chi}{2}\mathcal{H}_h(\tilde{f}(\alpha_i)D_h\dot{\alpha}_{0i}) + A_0(\dot{\theta}_i) + A_{-s}(\dot{\sigma}) \\ &+ \mathrm{O}(\dot{\zeta}_c) + \mathrm{O}(h^s),\end{aligned} \tag{9.59}$$

which give the variation of the normal and tangential velocities in terms of $\dot{\theta}$, $\dot{\sigma}$, $\dot{\alpha_0}$ and $\dot{\zeta}_c$, and is the main result of the section.

We next consider the variation of the surface tension $\dot{\mathcal{S}}$. It is easily seen from Equation (4.29) and Lemmas 8.0.11 and 8.0.12, that

$$\dot{\mathcal{S}}_i = \frac{1+\mathcal{S}_0(\alpha_i)}{s_{0\alpha}\alpha_{0\alpha}(\alpha_i)}\dot{\sigma} - \frac{s_\alpha(1+\mathcal{S}_0(\alpha_i))}{s_{0\alpha}\alpha_{0\alpha}^2(\alpha_i)}D_h\dot{\alpha}_0 + \dot{\mathcal{S}}_i^{NL} + \mathrm{O}(h^s), \tag{9.60}$$

where we have assumed $\dot{\mathcal{S}}_0 = 0$, i.e., the initial tension $\mathcal{S}_{0i}$ is exactly $\mathcal{S}_0(\alpha_i)$, and similarly $\dot{\sigma}_0 = 0$. An estimate for $\dot{\mathcal{S}}_i^{NL}$ is obtained by noting that

$$\begin{aligned}
\dot{\mathcal{S}}_i^{NL} &= \mathrm{O}(\dot{\sigma}^2 + (D_h\dot{\alpha}_0)^2), \\
&= h^3 A_{-s}(\dot{\sigma}) + h^2 A_0(D_h\dot{\alpha}_0), \\
&= A_{-s}(\dot{\sigma}) + A_{-1}(\dot{\alpha}_0),
\end{aligned} \tag{9.61}$$

where we have used $\|\dot{\sigma}\|_\infty, \|\dot{\sigma}_0\|_\infty \leq h^3$ and $\|D_h(\dot{\alpha}_0)\|_\infty \leq ch^2$. It follows that Equation (9.60) can be written as

$$\dot{\mathcal{S}}_i = A_{-s}(\dot{\sigma}) - \tilde{f}(\alpha_i) D_h \dot{\alpha}_0 + \mathrm{O}(h^s), \tag{9.62}$$

where

$$\tilde{f}(\alpha) = \frac{s_\alpha(1 + \mathcal{S}_0(\alpha))}{s_{0\alpha}\alpha_{0\alpha}^2(\alpha)} \tag{9.63}$$

is a smooth, real and positive function. The positivity the $\tilde{f}(\alpha)$ will be seen to be critical. Indeed, it is found to be necessary for the well-posedness of the continuous equations. We note that $\tilde{f}(\alpha_i)D_h\dot{\alpha}_0 = A_0(D_h\dot{\alpha}_0)$, but for later use we retain the specific form in (9.62).

The next quantity we need to estimate is the variation of ϕ_s. Recall the discrete equation for ϕ_s given by Equation (4.28). Taking the variation of this equation, we find

$$\begin{aligned}
(\dot{\phi}_s)_i = {} & S_h^{-1}\big(\dot{u_n}\theta_\alpha(\cdot) + u_n(\cdot)S_h\dot{\theta} - \langle \dot{u_n}\theta_\alpha(\cdot) + u_n(\cdot)S_h\dot{\theta}\rangle_h\big)_i \\
& + \mathrm{O}(h^s) + (\dot{\phi}_s^{NL})_i,
\end{aligned} \tag{9.64}$$

where

$$(\dot{\phi}_s^{NL})_i = S_h^{-1}\big(\dot{u_n}S_h\dot{\theta} - \langle \dot{u_n}S_h\dot{\theta}\rangle_h\big), \tag{9.65}$$

and recall the $O(h^s)$ term comes from, e.g., replacing $u_{nh}(\cdot)$ with $u_n(\cdot)$. We readily obtain from Lemma 8.0.19, Lemma 8.0.20 and Equation (9.58), the estimate

$$(\dot{\phi}_s)_i = A_0(S_h\dot{\theta}_i) + A_{-2}(\dot{\alpha}_{0i}) + A_{-s}(\dot{\sigma}) + O(\dot{\zeta}_c) + O(h^s). \tag{9.66}$$

In obtaining this estimate, we have used $A_{-1}(S_h^2\dot{\theta}) = A_0(S_h\dot{\theta})$, and the nonlinear terms have been estimated using $\|S_h\dot{\theta}\|_\infty \leq \frac{1}{h}\|\dot{\theta}\|_\infty \leq h^2$ and Equation (9.58), and are found to be smoother than terms already present in (9.66).

In order to complete the estimates, an estimate of $\dot{\omega}$ is required.

9.4 Leading Order Variation Of ω

For the case of viscosity matched fluids, in which $\beta = 0$ and $\chi = \frac{1}{2}$, the integral term in the continuous equation for ω (or equivalently the alternate point trapezoidal rule sum in the discrete equation) drops out, and the equation localizes. From Equation (4.8) with $\beta = 0$ and $\chi = \frac{1}{2}$, it is easy to see that

$$\begin{aligned}\dot{\omega}_i &= -\frac{1}{4}\big(\dot{\mathcal{S}}_i e^{i\theta(\alpha_i)} + \mathcal{S}(\alpha_i)(e^{i\theta})^{\cdot}_i\big) \\ &+ \frac{\kappa_B}{4s_\alpha^2}\big[i\theta_{\alpha\alpha}(\alpha_i)(e^{i\theta})^{\cdot}_i + ie^{i\theta(\alpha_i)}S_h^2\dot{\theta}_i\big] \\ &+ \frac{\kappa_B}{2s_\alpha} ie^{i\theta(\alpha_i)}\theta_{\alpha\alpha}(\alpha_i)\big(\frac{1}{\sigma}\big)^{\cdot}_i \\ &+ \dot{\omega}_i^{NL},\end{aligned} \tag{9.67}$$

where $\dot{\omega}_i^{NL}$ contains nonlinear terms in the variations $\left(\frac{1}{\sigma}\right)^{\cdot}_i$, $(e^{i\theta})^{\cdot}_i$, $\dot{\mathcal{S}}_i$, and discrete derivatives $S_h\dot{\theta}$ and $S_h^2\dot{\theta}$. We now give estimates for each of the terms in (9.67). Lemma 8.0.15 will provides the estimate (taking σ as one),

$$(e^{i\theta})^{\cdot}_i = ie^{i\theta(\alpha_i)}\dot{\theta}_i + A_{-3}(\dot{\theta}). \tag{9.68}$$

The variation $\dot{\mathcal{S}}$ is given in Equation (9.60). An estimate on the nonlinear term,

$$\dot{\omega}_i^{NL} = A_{-1}(\dot{\theta}) + A_{-s}(\dot{\sigma}) + O(h^2\dot{\zeta}_c) + O(h^s) \tag{9.69}$$

is derived below. We also need the following estimate for $\left(\frac{1}{\sigma}\right)^{\cdot}_i$.

Lemma 9.4.1. *Assume that* $\|\dot{\sigma}\|_{l^2} \leq h^{\frac{7}{2}}$ *and* $s_\alpha > a > 0$ *for some positive constant* a. *Then*

$$\left(\frac{1}{\sigma}\right)^{\cdot} = -\frac{\dot{\sigma}}{s_\alpha^2} + \frac{\dot{\sigma}^2}{s_\alpha^2\big(s_\alpha + \dot{\sigma}\big)}, \tag{9.70}$$

We also have

$$\left(\frac{1}{\sigma}\right)^{\cdot} = O(h^3), \tag{9.71}$$

and

$$f(\alpha_i)\left(\frac{1}{\sigma}\right)^{\cdot} = A_{-s}(\dot{\sigma}) \text{ for smooth } f. \tag{9.72}$$

Proof. We have from Lemma 8.0.12,

$$\left(\frac{1}{\sigma}\right)^{\cdot} = -\frac{\dot{\sigma}}{s_\alpha^2} + \frac{\dot{\sigma}^2}{s_\alpha^2\big(s_\alpha + \dot{\sigma}\big)}, \tag{9.73}$$

which gives (9.70). Relation (9.71) follows from (9.70) the boundedness s_α away from zero, and $\|\dot{\sigma}\|_\infty < h^3$. □

Together, Equations (9.67), (9.69), (9.60) and the above comments tell us that

$$\dot{\omega}_i = \kappa_B \frac{ie^{i\theta(\alpha_i)}}{4s_\alpha^2} S_h^2 \dot{\theta}_i + A_0(\dot{\theta}_i) + A_{-s}(\dot{\sigma}) + \frac{1}{4} e^{i\theta(\alpha_i)} \tilde{f}(\alpha_i)(S_h \dot{\alpha_0})_i + \mathrm{O}(h^2 \dot{\zeta}_c) + \mathrm{O}(h^s), \tag{9.74}$$

where $\tilde{f}(\alpha)$ is given by Equation (9.63). This further implies that:

$$A_{-2}(\dot{\omega}) = A_0(\dot{\theta}) + A_{-s}(\dot{\theta}) + A_{-1}(\dot{\alpha_0}) + h^2 \dot{\zeta}_c + \mathrm{O}(h^s), \tag{9.75}$$

and therefore $A_{-2}(\dot{\omega}^p)$ can be replaced with $A_{-1}(\dot{\alpha_0})$ in Equations (9.45), (9.56), (9.57), which leads to Equations (9.58), (9.59). We note that there are no $A_0(S_h\dot{\theta})$

terms in Equation (9.74), since these have canceled out. This will lead to an important simplification in the energy estimates developed later.

We complete the derivation of Equation (9.74) by giving details of the estimate (Equation (9.69)) for the nonlinear term $\dot{\omega}_i^{\mathrm{NL}}$. This term contains products of the form $(e^{-i\theta})^{\cdot}_i \dot{\mathcal{S}}_i$, $(e^{-i\theta})^{\cdot}_i S_h^p \dot{\theta}_i$ for $p = 1, 2$, $(S_h \dot{\theta}_i)^2$, $\dot{\left(\frac{1}{\sigma}\right)}(S_h \dot{\theta}_i)$, etc. We use $(e^{-i\theta})^{\cdot}_i = \mathrm{O}(h^3)$ (see Lemma 8.0.15) to obtain

$$(e^{-i\theta})^{\cdot}_i S_h^p \dot{\theta}_i = h^3 A_0(S_h^p \dot{\theta}_i) = A_{p-3}(\dot{\theta}) \tag{9.76}$$

for $p = 1, 2$. Similarly, from Equation (9.62),

$$(e^{-i\theta})^{\cdot}_i \dot{\mathcal{S}}_i = A_{-s}(\dot{\sigma}_i) + A_{-2}(\dot{\alpha}_0) + \mathrm{O}(h^s), \tag{9.77}$$

and using $S_h \dot{\theta} = \mathrm{O}(h^2)$,

$$(S_h \dot{\theta}_i)^2 = A_{-1}(\dot{\theta}_i). \tag{9.78}$$

Also, from Equation (9.71),

$$\left(\frac{1}{\sigma}\right)^{\cdot}_i S_h \dot{\theta}_i = A_{-2}(\dot{\theta}_i). \tag{9.79}$$

where the latter equality we have used Equation (9.72). The estimate Equation (9.69) readily follows. This verifies Equation (9.74) which is the main result of this section.

CHAPTER 10

EVOLUTION EQUATIONS FOR THE ERROR

An evolution equation for $\dot{\theta}$ is formed by first substituting the exact solution s_α, $\theta(\alpha_i)$ into Equation (4.22), using consistency, and substracting the result from Equation (4.22). This gives

$$\begin{aligned}
\frac{d\dot{\theta}_i}{dt} &= \frac{1}{\sigma}\big[S_h(u_n)_i + (\phi_s)_i S_h \theta_i\big] \\
&- \frac{1}{s_\alpha}\big[S_h(u_n)_h(\alpha_i) + (\phi_s)_h(\alpha_i) S_h \theta(\alpha_i)\big] + \mathrm{O}(h^s) \\
&= \frac{1}{s_\alpha}\big(S_h(\dot{u_n})_i + \phi_s(\alpha_i) S_h(\dot{\theta}_i) + \theta_\alpha(\alpha_i)(\dot{\phi_s})_i\big) \\
&+ \frac{1}{\dot{\sigma}}\big((u_n)_\alpha(\alpha_i) + \phi_s(\alpha_i)\theta_\alpha(\alpha_i)\big) \\
&+ \Theta_i^{\mathrm{NL}} + \mathrm{O}(h^s),
\end{aligned} \tag{10.1}$$

where the nonlinear term Θ_i^{NL} contains products of the variations. In (10.1), we have also used consistency to replace, for example, $S_h(\theta(\alpha_i))$ with $\theta_\alpha(\alpha_i)$, incurring an $\mathrm{O}(h^s)$ error. It is easy to see from Equations (9.59), (9.66) and Lemma 9.4.1 that the nonlinear terms satisfies

$$\dot{\Theta}_i^{\mathrm{NL}} = A_0(\dot{\theta}) + A_{-s}(\dot{\sigma}) + \mathrm{O}(h^3\dot{\zeta}_c) + \mathrm{O}(h^s), \tag{10.2}$$

where for the leading order part, we have used the estimate

$$\begin{aligned}
\left(\frac{1}{\sigma}\right)_i^{\cdot}(S_h(u_n))_i^{\cdot} &= \mathrm{O}(h^3)\big(S_h A_0(S_h^2\dot{\theta}) + A_{-s}(\dot{\sigma}) + \mathrm{O}(\dot{\zeta}_c) + \mathrm{O}(h^s)\big) \\
&= A_0(\dot{\theta}) + A_{-s}(\dot{\sigma}) + \mathrm{O}(h^3\dot{\zeta}_c) + \mathrm{O}(h^s).
\end{aligned} \tag{10.3}$$

The relation (Equation (10.1)) can be further simplified using Equations (9.58), (9.66) and Lemma 9.4.1, which give

$$\frac{d\dot{\theta}_i}{dt} = \frac{\kappa_B}{4s_\alpha^3}\mathcal{H}_h(S_h^3\dot{\theta}_i) + S_hA_0(\dot{\theta}_i) + A_0(S_h\dot{\theta}_i) + S_hA_{-1}(\dot{\alpha}_{0i})$$
$$+ A_{-s}(\dot{\sigma}) + \mathrm{O}(\dot{\zeta}_c) + \mathrm{O}(h^s), \tag{10.4}$$

In deriving Equation (10.4), we have made use of the fact that $\dot{\zeta}_c$ is spatially independent and can be pulled outside of a spatial operator.

The evolution equation for $\dot{\sigma}$ is derived similarly. We substitute the exact solution into Equation (4.23), use consistency, and substract the result from Equation (4.23) to obtain

$$\begin{aligned}\frac{d\dot{\sigma}}{dt} &= -\langle u_n S_h\theta\rangle_h + \langle (u_n)_h(\cdot)S_h\theta(\cdot)\rangle + \mathrm{O}(h^s)\\ &= -\langle (\dot{u_n})\theta_\alpha(\cdot)\rangle_h - \langle u_n(\cdot)S_h\dot{\theta}\rangle_h - \langle (\dot{u_n})S_h\dot{\theta}\rangle_h + \mathrm{O}(h^s).\end{aligned} \tag{10.5}$$

The nonlinear term is estimated as

$$\langle (\dot{u_n})S_h\dot{\theta}\rangle_h = A_0(\dot{\theta}) + A_{-s}(\dot{\sigma}) + \mathrm{O}(h^2\dot{\zeta}_c) + \mathrm{O}(h^s), \tag{10.6}$$

using Equation (9.56) and the bound $\|S_h\dot{\theta}\|_{l^2} \leq h^2$. Equation (10.5) can be further simplified using Lemmas 8.0.14−8.0.16, which together with (10.6) gives

$$\frac{d\dot{\sigma}_i}{dt} = A_0(\dot{\theta}) + A_{-s}(\dot{\sigma}) + \mathrm{O}(\dot{\zeta}_c) + \mathrm{O}(h^s). \tag{10.7}$$

We also need the variation of the evolution Equation (4.30) for $\dot{\alpha}_0$. Let

$$u_t(\alpha) = (\phi_s(\alpha) - u_s(\alpha))e^{i\theta(\alpha)} \tag{10.8}$$

be the difference between the tangential interface velocity at a fixed α and the tangential fluid velocity at $\tau(\alpha)$. Taking the variation of Equation (4.30) gives

$$\left(\frac{d\dot{\alpha}_0}{dt}\right)_i = \frac{u_t(\alpha_i)}{s_\alpha e^{i\theta(\alpha_i)}}(D_h\dot{\alpha}_0)_i - \frac{\alpha_{0\alpha}(\alpha_i)u_t(\alpha_i)}{s_\alpha^2 e^{i\theta(\alpha_i)}}\dot{\sigma} - \frac{\alpha_{0\alpha}(\alpha_i)u_t(\alpha_i)}{s_\alpha(e^{i\theta(\alpha_i)})^2}(e^{i\theta_i})^{\cdot}$$
$$+ \frac{\alpha_{0\alpha}(\alpha_i)}{s_\alpha e^{i\theta(\alpha_i)}}(\dot{u}_t)_i + (\dot{\alpha_0}^{NL})_i + \mathrm{O}(h^s), \tag{10.9}$$

where $\dot{\alpha_0}^{NL}$ contains the nonlinear terms, which can be compactly represented as

$$\dot{\alpha}_{0i}^{NL} = \mathrm{O}\big((S_h\dot{\alpha}_0)^2 + \dot{\sigma}^2 + (e^{i\theta})^{\cdot 2} + (\dot{u}_t)^2\big)_i \tag{10.10}$$

From Equations (9.59) and (9.66), we have (taking $\chi = \frac{1}{2}$),

$$(u_t)^{\cdot}_i = -\frac{e^{-i\theta(\alpha_i)}}{4}\mathcal{H}_h\big(\tilde{f}(\alpha_i)D_h\dot{\alpha}_{0i}\big) + A_0(S_h\dot{\theta}_i) + A_{-s}(\dot{\sigma}) + A_{-1}(\dot{\alpha}_{0i})$$
$$+ \mathrm{O}(\dot{\zeta}_c) + \mathrm{O}(h^s), \tag{10.11}$$

where we have also used Lemma 8.0.15. Define the smooth functions

$$\tilde{f}_1(\alpha) = \frac{u_t(\alpha)}{s_\alpha e^{i\theta(\alpha)}} \text{ and } \tilde{f}_2(\alpha) = \frac{\tilde{f}(\alpha)(\alpha_0)_\alpha(\alpha)}{4s_\alpha}, \tag{10.12}$$

where importantly $\alpha_{0\alpha}(\alpha)$ and hence $\tilde{f}_2(\alpha)$ are both positive functions. We note that $\alpha_{0\alpha}(\alpha) = 1$ at $t = 0$, and the positive definiteness of $\alpha_{0\alpha}$ is a consequence of $\alpha_0(\alpha)$ being a one-to-one mapping, which is related to the physical property that material fluid points cannot overlap. Using (10.11) and (10.12), Equation (10.9) can be written

$$\left(\frac{d\dot{\alpha}_0}{dt}\right)_i = \tilde{f}_1(\alpha_i)(D_h\dot{\alpha}_0)_i - \tilde{f}_2(\alpha_i)\mathcal{H}_h D_h\dot{\alpha}_{0i} + A_0(S_h\dot{\theta}_i)$$
$$+ A_{-s}(\dot{\sigma}) + A_{-1}(\dot{\alpha}_{0i}) + \mathrm{O}(\dot{\zeta}_c) + \mathrm{O}(h^s). \tag{10.13}$$

The nonlinear terms are smoother or smaller than terms that are already present in (10.13), as is easily verified by reader.

Next, we derive the evolution equation for $\dot{\zeta}_c$. We have defined ζ_c as the $k = 0$ Fourier mode of the discrete interface ζ_i. Recall the evolution equation for ζ_c is

Equation (4.27),

$$\left.\frac{d\zeta_c}{dt}\right|_{\alpha} = \hat{v}_0. \tag{10.14}$$

It immediately follows that

$$\left.\frac{d\dot{\zeta}_c}{dt}\right|_{\alpha} = \hat{\dot{v}}_0 \tag{10.15}$$

is the evolution equation for $\dot{\zeta}_c$. Equations (10.4), (10.7), (10.13), and (10.15) are the main results of the chapter.

CHAPTER 11

ENERGY ESTIMATES

We first recall that we have defined a time:

$$T^* \equiv \sup\big\{t : 0 \le t \le T, \|\dot{\sigma}\|_{l^2}, \|\dot{\theta}\|_{l^2}, \|\dot{\zeta}\|_{l^2}, \|\dot{\alpha_0}\|_{l^2} \le h^{\frac{7}{2}}\big\}. \tag{11.1}$$

The power of h in the above definition is chosen for convenience, so that the estimates below easily go through. All the estimates we obtain are valid for $t \le T^*$. We "close the argument" and prove Theorem 7.0.2 by showing at the end that $T^* = T$. Define the energy

$$E(t) = \dot{\sigma}^2 + \big(\dot{\theta}, \dot{\theta}\big)_h + \big(\dot{\alpha_0}, \dot{\alpha_0}\big)_h + |\dot{\zeta}_c|^2, \tag{11.2}$$

where we recall $(f,g)_h$ is the inner product $h \displaystyle\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} f_i g_i$. Take the time derivative of E and use Equations (10.4), (10.7) to obtain

$$\begin{aligned}
\frac{1}{2}\frac{dE}{dt} &= \dot{\sigma}\dot{\sigma}_t + \big(\dot{\theta}, \dot{\theta}_t\big)_h + \big(\dot{\alpha_0}, \dot{\alpha}_{0t}\big)_h + 2\mathrm{Re}\big(\overline{\dot{\zeta}_c}\dot{\zeta}_{ct}\big), \\
&= \dot{\sigma}\big(A_0(\dot{\theta}) + A_{-s}(\dot{\sigma}) + \mathrm{O}(|\dot{\zeta}_c|) + \mathrm{O}(h^s)\big) \\
&+ \Big(\dot{\theta}, \frac{\kappa_B}{4s_\alpha^3}\mathcal{H}_h(S_h^3\dot{\theta}) + S_h A_0(\dot{\theta}) + A_0(S_h\dot{\theta}) \\
&+ A_{-s}(\dot{\sigma}) + \mathrm{O}(\dot{\zeta}_c) + \mathrm{O}(h^s)\Big)_h \\
&+ \big(\dot{\alpha_0}, \dot{\alpha}_{0t}\big)_h + 2\mathrm{Re}\big(\overline{\dot{\zeta}_c}\dot{\zeta}_{ct}\big).
\end{aligned} \tag{11.3}$$

The first product on the right side of (11.3) is readily bounded using Young's inequality:

$$\dot{\sigma}\big(A_0(\dot{\theta}) + A_{-s}(\dot{\sigma}) + \mathrm{O}(|\dot{\zeta}_c|) + \mathrm{O}(h^s)\big) \le cE + \mathrm{O}(h^s). \tag{11.4}$$

We bound the inner product in Equation (11.3) by making use of parabolic smoothing. The first term in this inner product is evaluated as

$$\left(\dot{\theta}, \frac{\kappa_B}{4s_\alpha^3}\mathcal{H}_h(S_h^3\dot{\theta}_i)\right)_h = -\frac{\kappa_B}{4s_\alpha^3}\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}-1}|k|^3|\hat{\dot{\theta}}_k|^3, \tag{11.5}$$

where we have used the discrete Parseval's equality (Lemma 8.0.18), Equation (8.17), and the real valuedness of $\dot{\theta}$ (so that $|\hat{\dot{\theta}}_k| = |\hat{\dot{\theta}}_{-k}|$). The sum extends to $k = \frac{N}{2} - 1$, in view of zeroing out the $\frac{N}{2}$ mode of $S_h\dot{\theta}$. The next term is bounded using Parseval's equality and Young's inequality:

$$\begin{aligned}
\left|\left(\dot{\theta}, S_h(A_0(\dot{\theta}))\right)_h\right| &= \left|\left(S_h\dot{\theta}, A_0(\dot{\theta})\right)_h\right| \\
&\leq \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}-1}|k||\hat{\dot{\theta}}_k||\widehat{(A_0(\dot{\theta}))}_k|, \\
&\leq \frac{1}{2}\left[\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}-1}\left(k^2|\hat{\dot{\theta}}_k|^2 + |\widehat{(A_0(\dot{\theta}))}_k|^2\right)\right], \\
&\leq c\left(E + \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}-1}k^2|\hat{\dot{\theta}}_k|^2\right),
\end{aligned} \tag{11.6}$$

for a constant c. In the last inequality, we have used

$$\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}-1}|\widehat{(A_0(\dot{\theta}))}_k|^2 \leq \|A_0(\dot{\theta})\|_{l^2}^2 \leq c\|\dot{\theta}\|_{l^2}^2 = c\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}-1}|\hat{\dot{\theta}}_k|^2. \leq cE \tag{11.7}$$

We similarly bound

$$\begin{aligned}
\left|\left(\dot{\theta}, A_0(S_h\dot{\theta})\right)_h\right| &\leq \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}-1}|\hat{\dot{\theta}}_k||\widehat{(A_0(S_h\dot{\theta}))}_k| \\
&\leq \frac{1}{2}\left[\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}-1}\left(|\hat{\dot{\theta}}_k|^2 + |\widehat{(A_0(S_h\dot{\theta}))}_k|^2\right)\right] \\
&\leq c\left(E + \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}-1}k^2|\hat{\dot{\theta}}_k|^2\right),
\end{aligned} \tag{11.8}$$

where $c > 0$ and the last inequality follows from the bound

$$\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}-1} |(\widehat{A_0(S_h\dot{\theta})})_k|^2 \le \|A_0(S_h\dot{\theta})\|_{l^2}^2 \le c\|S_h\dot{\theta}\|_{l^2}^2 = c\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}-1} k^2|\hat{\dot{\theta}}_k|^2. \tag{11.9}$$

For the next three terms in Equation (11.3), we use the bound

$$\left|\big(\dot{\theta}, A_{-s}(\dot{\sigma}) + \mathrm{O}(\dot{\zeta}_c) + \mathrm{O}(h^s)\big)_h\right| \le cE + \mathrm{O}(h^s). \tag{11.10}$$

Next, we estimate the inner product $(\dot{\alpha}_{0t}, \dot{\alpha}_0)_h$ in Equation (11.3). We substitute Equation (10.13) for $\dot{\alpha}_{0t}$ to obtain

$$\begin{aligned}\big(\dot{\alpha}_{0t}, \dot{\alpha}_0\big)_h = \big(\tilde{f}_1(\cdot)D_h\dot{\alpha}_0, \dot{\alpha}_0\big)_h - \big(\tilde{f}_2(\cdot)\mathcal{H}_h(D_h\dot{\alpha}_0), \dot{\alpha}_0\big)_h + \big(A_0(S_h\dot{\theta})\\ + A_{-s}(\dot{\sigma}) + A_{-1}(\dot{\alpha}_0) + \mathrm{O}(\dot{\zeta}_c), \dot{\alpha}_0\big)_h + \mathrm{O}(h^s).\end{aligned} \tag{11.11}$$

The first inner product on the right hand side of (11.11), which can be written $\big(\tilde{f}_1(\cdot)\dot{\alpha}_0, D_h\dot{\alpha}_0\big)_h$, is estimated using the discrete Parseval's equality and Lemma 8.0.10 as

$$\begin{aligned}\big(\tilde{f}_1(\cdot)\dot{\alpha}_0, D_h\dot{\alpha}_0\big)_h &= -\big(D_h(\tilde{f}_1(\cdot)\dot{\alpha}_0), \dot{\alpha}_0\big)_h\\ &= -\big(\tilde{f}_1(\cdot)D_h\dot{\alpha}_0 + \dot{\alpha}_0^q\tilde{f}_{1\alpha}(\cdot) + hA_0(\dot{\alpha}_0), \dot{\alpha}_0\big)_h.\end{aligned} \tag{11.12}$$

Move the first inner product on the right hand side of (11.12) to the left hand side (also moving the real function $\tilde{f}_1$ to the other side of the inner product) to obtain

$$2\big(\tilde{f}_1(\cdot)\dot{\alpha}_0, D_h\dot{\alpha}_0\big)_h = -\big(\dot{\alpha}_0^q\tilde{f}_{1\alpha}(\cdot) + hA_0(\dot{\alpha}_0), \dot{\alpha}_0\big)_h. \tag{11.13}$$

This shows that the inner product is bounded by the energy, i.e.,

$$\left|\big(\tilde{f}_1(\cdot)\dot{\alpha}_0, D_h\dot{\alpha}_0\big)_h\right| \le cE. \tag{11.14}$$

The second inner product on the right hand side of (11.11) can be written $-\big(\Lambda_h^p\dot{\alpha}_0, \tilde{f}_2(\cdot)\dot{\alpha}_0\big)_h$, where we have defined $\Lambda_h^p = \mathcal{H}_hD_h$. To bound this inner product, we make essential use of the positive definiteness of $\tilde{f}_2$. We first write:

$$-\big(\Lambda_h^p\dot{\alpha}_0, \tilde{f}_2(\cdot)\dot{\alpha}_0\big)_h = -\big(\sqrt{\tilde{f}_2(\cdot)}\Lambda_h^p\dot{\alpha}_0, \sqrt{\tilde{f}_2(\cdot)}\dot{\alpha}_0\big)_h, \tag{11.15}$$

then move $\sqrt{\tilde{f}_2(\cdot)}$ inside the argument of the operator Λ_h^p, which by Lemma 8.0.8 and the discrete product rule Lemma 8.0.10 introduces a commutator and other terms whose inner product with α_0 can be bounded by energy. If we define $\dot{\tilde{\alpha}}_0 = \sqrt{\tilde{f}_2(\cdot)}\dot{\alpha}_0$, then the preceding statements imply that

$$-\big(\sqrt{\tilde{f}_2(\cdot)}\Lambda_h^p\dot{\alpha}_0, \sqrt{\tilde{f}_2(\cdot)}\dot{\alpha}_0\big)_h = -\big(\Lambda_h^p\dot{\tilde{\alpha}}_0, \dot{\tilde{\alpha}}_0\big)_h + r \tag{11.16}$$

where $r \in \mathbb{R}$ satisfies $|r| < cE$. The inner product on the right hand side of (11.16) satisfies

$$\big(\Lambda_h^p\dot{\tilde{\alpha}}_0, \dot{\tilde{\alpha}}_0\big)_h = \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} |k|\rho(kh)|\dot{\tilde{\alpha}}_0|^2 > 0. \tag{11.17}$$

Combining (11.15)-(11.17) shows that

$$\big(\Lambda_h^p\dot{\alpha}_0, \tilde{f}_2(\cdot)\dot{\alpha}_0\big)_h \leq cE, \tag{11.18}$$

which gives the desired estimate on the second inner product in Equation (11.11).

The third inner product that we need to estimate is $\big(A_0(S_h\dot{\theta}), \dot{\alpha}_0\big)_h$. This is bounded using Young's inequality as

$$\begin{aligned}
\big|\big(A_0(S_h\dot{\theta}), \dot{\alpha}_0\big)_h\big| &\leq \frac{1}{2}\big(\|A_0(S_h\dot{\theta})\|_{l^2}^2 + \|\dot{\alpha}_0\|_{l^2}^2\big), \\
&\leq c\big(\|S_h\dot{\theta}\|_{l^2}^2 + \|\dot{\alpha}_0\|_{l^2}^2\big), \\
&\leq c\Big(\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}-1} |k|^2|\hat{\dot{\theta}}_k|^2 + E\Big).
\end{aligned} \tag{11.19}$$

The first sum above will be controlled by parabolic smoothing (i.e., by the dominant contribution from the leading order term Equation (11.5)). The second sum above is bounded by the energy.

The other inner products in Equation (11.11) are clearly bounded by cE. Putting these estimates together, we have obtained the bound

$$\big(\dot{\alpha}_{0t}, \dot{\alpha}_0\big)_h \le c\Big(\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}-1} |k|^2 |\hat{\dot{\theta}}_k|^2 + E\Big) + \mathrm{O}(h^s). \tag{11.20}$$

The final term in Equation (11.3) is estimated using Equation (10.15) and Young's inequality as

$$\begin{aligned} 2|\mathrm{Re}\big(\overline{\dot{\zeta}_c}\dot{\zeta}_{ct}\big)| &\le 2|\dot{\zeta}_c||\dot{\zeta}_{ct}|, \\ &\le 2|\dot{\zeta}_c||\widehat{\dot{v}}_0|, \\ &\le |\dot{\zeta}_c|^2 + |\widehat{\dot{v}}_0|^2, \\ &\le |\dot{\zeta}_c|^2 + \|\widehat{\dot{v}}\|_{l^2}^2. \end{aligned} \tag{11.21}$$

where we recall that $\dot{v} = \big(u_n i e^{i\theta} + \phi_s e^{i\theta}\big)^{\dot{}}$. From expressions for $\dot{u_n}$ and $\dot{\phi}_s$ given in Equations (9.58) and (9.66), it is easy to see that

$$\begin{aligned} \|\dot{v}\|_{l^2}^2 \le c\big(&\|S_h\dot{\theta}\|_{l^2}^2 + \|A_{-2}(\dot{\alpha}_0)\|_{l^2}^2 + |\dot{\zeta}_c|^2 + \|A_0(\dot{\theta})\|_{l^2}^2 \\ &+ \|A_{-s}(\dot{\sigma})\|_{l^2}^2 + \mathrm{O}(h^s)\big). \end{aligned} \tag{11.22}$$

Therefore,

$$2|\mathrm{Re}\big(\overline{\dot{\zeta}_c}\dot{\zeta}_{ct}\big)| \le c\Big(\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}-1} |k|^2 |\hat{\dot{\theta}}_k|^2 + cE + \mathrm{O}(h^s)\Big), \tag{11.23}$$

which gives the desired bound on the last term Equation (11.3).

We now put these estimates together. First, set

$$d_1 = \min_{0\le t\le T} \frac{\kappa_B}{2 s_\alpha}, \tag{11.24}$$

and note by assumptions on s_α that $0 < c_1 < d_1 < \infty$, so in particular d_1 is bounded away from zero. Then from Equations (11.5), (11.6), (11.7), (11.8), and (11.23), there exists positive constants d_2, d_3, such that Equation (11.3) can be bounded as

$$\frac{dE}{dt} \le \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}-1} \big(- d_1|k|^3 + d_2 k^2 \big) |\hat{\dot{\theta}}_k|^2 + d_3 E + \mathrm{O}(h^s). \tag{11.25}$$

Let $0 < \varepsilon < d_1$ be fixed. Then (11.25) can be written as

$$\frac{dE}{dt} \le \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}-1} d_4 |\hat{\dot{\theta}}_k|^2 + d_3 E + \mathrm{O}(h^s), \tag{11.26}$$

where

$$d_4 = \max_{-\frac{N}{2}+1 \le k \le \frac{N}{2}} \big(- d_1|k|^3 + d_2 k^2 \big), \tag{11.27}$$

(Note that $0 < d_4 < \infty$). It readily follows that there exists a positive constant c such that

$$\frac{dE}{dt} \le cE + \mathrm{O}(h^s), \text{ with } E(0) = 0 \tag{11.28}$$

for $t \le T^*$, which is the main result of this chapter.

Stability and convergence of our numerical method now follows from (11.28). Application of Gronwall's inequality to (11.28) gives

$$E(t) \le ch^s t(1 + e^t) \text{ for } t \le T^*, \tag{11.29}$$

or

$$E(t) \le c(T^*)h^s, \tag{11.30}$$

It follows that

$$\|\dot{\sigma}\|_{l^2}^2,\ \|\dot{\theta}\|_{l^2}^2,\ \|\dot{\alpha}_0\|_{l^2}^2,\ \|\dot{\zeta}\|_{l^2}^2 \le c(T^*)h^s, \tag{11.31}$$

where we have used $\|\dot{\zeta}\|_{l^2}^2 \leq cE$, which follows from Lemma 8.0.16 and $\|\dot{\zeta}_c\|_{l^2}^2 \leq cE$. We choose m large enough, so that s can be picked to satisfy $s \geq 8$. (Recall that m characterizes the smoothness of the continuous solution, and s is near m). Then

$$\|\dot{\sigma}\|_{l^2},\ \|\dot{\theta}\|_{l^2},\ \|\dot{\alpha}_0\|_{l^2},\ \|\dot{\zeta}\|_{l^2} \leq c(T^*)h^{\frac{s}{2}} < h^{\frac{7}{2}} \tag{11.32}$$

for h small enough. We can therefore extend T^* to $T^* = T$, so that the bounds (11.32) are valid throughout the entire interval $0 \leq t \leq T$ in which a smooth continuous solution exists. This completes the proof of the convergence of our method for $\beta = 0$, $\chi = \frac{1}{2}$ and $\kappa_B > 0$.

CHAPTER 12

CONCLUSIONS

A convergence proof has been presented for a boundary integral method for interfacial Stokes flow. While previous convergence analyses of the boundary integral method exist for interfacial potential flow, this is the first analysis that we are aware of for the important case of interfacial Stokes flow. Our analysis has focused on a spectrally accurate numerical method, adapted in this research from [22], for a Hookean elastic capsule with membrane bending stress evolving in an externally applied strain or shear flow. The method is based on an arclength-angle parametrization of the interface which was introduced in [25] to remove numerical stiffness in an efficient manner.

The main task in the proof is to estimate the variations or errors $\dot{\theta} = \theta_i - \theta(\alpha_i)$, $\dot{\sigma} = \sigma - s_\alpha$ between the discrete and exact solutions at time t. This is done by estimating the most singular terms in the variations, and seperating into linear and nonlinear terms in $\dot{\theta}$, $\dot{\sigma}$. The nonlinear terms are controlled by the high (spectral) accuracy of the method for smooth solutions, and thus the crux of the proof is show the stability of the linear terms in the variation, which is done with the aid of energy estimates.

The presence of high derivatives due to the bending forces requires a substantially different analysis from previous proofs of the convergence of the boundary integral method for potential flow. In particular, our energy estimate make significant use of the smoothing properties of the highest derivative term, or so-called 'parabolic smoothing', to control lower order derivatives. This allows us to close the energy estimates and prove stability of the method.

The proof also clarifies the role of numerical filtering in the particular boundary integral method analyzed in this research. We find that targeted filtering is necessary to control the potentially destabilizing effect of aliasing errors and prove stability of the method. Crucially, however, our analysis shows that the filter should not be applied to the highest derivative term coming from the membrane bending stress, so that the smoothing properties of this term can utilized.

In future work, we shall consider the convergence analysis of the boundary integral method for drops and bubbles without a surrounding elastic membrane. In this case, the interfacial tension $\mathcal{S}$ is constant in space and the bending stress κ_B is zero. We may also consider the convergence analysis for an inextensible membrane, in which $\mathcal{S}$ is determined by enforcing the surface divergence of the interfacial velocity to be zero, i.e.,

$$\mathbf{x}_s \cdot \mathbf{u}_s(\mathbf{x}) = 0, \text{ for } x \in \gamma \tag{12.1}$$

In other future work, we may also consider the convergence of recent algorithms, e.g., [33], in which artificial contact forces are introduced to prevent fluid drops or vesicles from coming into close contact. Since the contact forces act over a small region that scales with the grid size, it is expected that methods utilizing these forces converge to solutions of the continuous equations (without contact forces). However, no proof or demonstration of convergence currently exists.

APPENDIX A

PROOF OF LEMMAS

Proof. Proof of Lemma 8.0.20 Define:

$$\hat{f}_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(\alpha)e^{-ik\alpha}d\alpha, \tag{A.1}$$

and let:

$$\hat{F}_k = \sum_{m=-\infty}^{\infty} \hat{f}_{k+mN} \text{ for } -\frac{N}{2}+1 \leq k \leq \frac{N}{2} \tag{A.2}$$

denote the discrete Fourier coefficients of f, taking aliasing into account. Thus:

$$f(\alpha_i) = \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} \hat{F}_k e^{ik\alpha_i}, \tag{A.3}$$

$$\phi_i = \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} \hat{\phi}_k e^{ik\alpha_i}. \tag{A.4}$$

$$\tag{A.5}$$

Our interest is in obtaining an estimate for:

$$S_h^{-1}(f(\cdot)S_h\phi)_i = \sum_{\substack{k=-\frac{N}{2}+1 \\ k\neq 0}}^{\frac{N}{2}} \frac{1}{ik}(\widehat{fS_h\phi})_k e^{ik\alpha_i}, \tag{A.6}$$

where $(\widehat{fS_h\phi})_k$ denotes the discrete Fourier coefficients of the product $fS_h\phi$.

As a preliminary, we shall need an expression for the Fourier coefficients of the product of a smooth function with a discrete function. For a given k, define the sets:

$$\begin{aligned} I_{n,k} &= \left\{ n \in \mathbb{Z} : -\frac{N}{2} + 1 \leq k - n \leq \frac{N}{2} \right\}, \\ J_{n,k} &= \left\{ n \in \mathbb{Z} : -\frac{N}{2} + 1 \leq k + N - n \leq \frac{N}{2} \right\}, \\ K_{n,k} &= \left\{ n \in \mathbb{Z} : -\frac{N}{2} + 1 \leq k - N - n \leq \frac{N}{2} \right\}. \end{aligned} \tag{A.7}$$

Using Equations (A.3) and (A.4), the product $f(\alpha_i)\phi_i$ can be written as:

$$f(\alpha_i)\phi_i = \left(\sum_{k=-N+2}^{-\frac{N}{2}} + \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} + \sum_{k=\frac{N}{2}+1}^{N} \right) \sum_{n \in I_{n,k}} \hat{F}_{k-n} \hat{\phi}_n e^{ik\alpha_i}, \tag{A.8}$$

where we use the notation $\sum_{n \in I_{n,k}}$ to represent $\sum_{\substack{n=-\frac{N}{2}+1 \\ n \in I_{n,k}}}^{\frac{N}{2}}$. Equivalently, $\hat{\phi}_n$ is set to zero for n outside the range $[-\frac{N}{2}+1, \frac{N}{2}]$ (this is known as 'zero padding'). The wave numbers in the first and third sums in parenthesis are aliased to $k \in [-\frac{N}{2}+1, \frac{N}{2}]$. Rewriting these two sums by replacing k with $k - N$ and $k + N$, respectively, we obtain the equivalent representation:

$$\begin{aligned} f(\alpha_i)\phi_i = \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} \Bigg(& \sum_{n \in I_{n,k}} \hat{F}_{k-n} \hat{\phi}_n + \sum_{n \in J_{n,k}} \hat{F}_{k+N-n} \hat{\phi}_n \\ & + \sum_{n \in K_{n,k}} \hat{F}_{k-N-n} \hat{\phi}_n \Bigg) e^{ik\alpha_i}, \end{aligned} \tag{A.9}$$

where the requirement $n \in J_{n,k}$ in the second double sum of (A.9) and $n \in K_{n,k}$ in the third has allowed us to replace $\sum_{k=-\frac{N}{2}+1}^{0}$ and $\sum_{k=2}^{\frac{N}{2}}$, respectively, with $\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}}$. For

Equation (A.9), we therefore have for $-\frac{N}{2}+1 \leq k \leq \frac{N}{2}$:

$$\widehat{(fS_h\phi)}_k = \sum_{n\in I_{n,k}} in\hat{F}_{k-n}\hat{\phi}_n + \sum_{n\in J_{n,k}} in\hat{F}_{k+N-n}\hat{\phi}_n + \sum_{n\in K_{n,k}} in\hat{F}_{k-N-n}\hat{\phi}_n. \tag{A.10}$$

and similarly,

$$\widehat{(\phi S_h f)}_k = \sum_{n\in I_{n,k}} i(k-n)\hat{F}_{k-n}\hat{\phi}_n + \sum_{n\in J_{n,k}} i(k+N-n)\hat{F}_{k+N-n}\hat{\phi}_n + \sum_{n\in K_{n,k}} i(k-N-n)\hat{F}_{k-N-n}\hat{\phi}_n. \tag{A.11}$$

Combining Equation (A.10) with the negative of Equation (A.11) gives for $-\frac{N}{2}+1 \leq k \leq \frac{N}{2}$:

$$\widehat{(fS_h\phi)}_k = -\widehat{(\phi S_h f)}_k + \sum_{n\in I_{n,k}} ik\hat{F}_{k-n}\hat{\phi}_n + \sum_{n\in J_{n,k}} i(k+N)\hat{F}_{k+N-n}\hat{\phi}_n + \sum_{n\in K_{n,k}} i(k-N)\hat{F}_{k-N-n}\hat{\phi}_n. \tag{A.12}$$

We next recognize from Equation (A.9) that:

$$\widehat{(f\phi)}_k = \sum_{n\in I_{n,k}} \hat{F}_{k-n}\hat{\phi}_n + \sum_{n\in J_{n,k}} \hat{F}_{k+N-n}\hat{\phi}_n + \sum_{n\in K_{n,k}} \hat{F}_{k-N-n}\hat{\phi}_n, \tag{A.13}$$

and combining this with Equation (A.11) shows that the Fourier coefficients in Equation (A.6) can be written as:

$$\frac{\widehat{(fS_h\phi)}_k}{ik} = -\frac{\widehat{(\phi S_h f)}_k}{ik} + \widehat{(f\phi)}_k + \sum_{n\in J_{n,k}} \frac{N}{k}\hat{F}_{k+N-n}\hat{\phi}_n - \sum_{n\in K_{n,k}} \frac{N}{k}\hat{F}_{k-N-n}\hat{\phi}_n, \tag{A.14}$$

for $-\frac{N}{2}+1 \leq k \leq \frac{N}{2}$ with $k \neq 0$. The first three terms in Equation (A.14) are the Fourier coefficients of the first three terms in Equation (8.52). To finish the derivation of Equation (8.52), we simply need to estimate the two sums on the right hand side of Equation (A.14). The main difficulty is to overcome the large factor of N.

Each of the two sums in Equation (A.14) is a discrete convolution which represents the k-th Fourier coefficient of the product a smooth function with ϕ_i. Denoting the smooth functions by f_1 and f_2, we form the l^2-norm of the products with the aid of the discrete Parseval equality (Lemma 8.0.18),

$$\|f_1(\cdot)\phi\|_{l^2} = \left(2\pi \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} \left(\sum_{n \in J_{n,k}} \frac{N}{k} \hat{F}_{k+N-n} \hat{\phi}_n \right)^2 \right)^{\frac{1}{2}}, \tag{A.15}$$

and

$$\|f_2(\cdot)\phi\|_{l^2} = \left(2\pi \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} \left(\sum_{n \in K_{n,k}} \frac{N}{k} \hat{F}_{k-N-n} \hat{\phi}_n \right)^2 \right)^{\frac{1}{2}}. \tag{A.16}$$

We estimate these l^2-norms by decomposing the wavenumber range into

$$\varkappa_1 = \left\{ k : \frac{N}{4} \leq |k| \leq \frac{N}{2} \right\}, \tag{A.17}$$

and

$$\varkappa_2 = \left\{ k : 0 < |k| < \frac{N}{4} \right\}. \tag{A.18}$$

The sum over $k \in \varkappa_1$ is bounded using $|\frac{N}{k}| \leq 4$. For example,

$$\begin{aligned}
&\left[2\pi \sum_{k\in\varkappa_1} \left(\frac{N}{k} \sum_{n\in J_{n,k}} \hat{F}_{k+N-n}\hat{\phi}_n\right)^2\right]^{\frac{1}{2}} \\
\leq& 4\left[2\pi \sum_{k\in\varkappa_1} \left(\sum_{n\in J_{n,k}} \hat{F}_{k+N-n}\hat{\phi}_n\right)^2\right]^{\frac{1}{2}} \\
\leq& 4\left[2\pi \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} \left(\sum_{n\in J_{n,k}} \hat{F}_{k+N-n}\hat{\phi}_n\right)^2\right]^{\frac{1}{2}}, \qquad \text{(A.19)} \\
=& 4\left[2\pi \sum_{k=\frac{N}{2}+1}^{N} \sum_{n\in I_{n,k}} \left(\hat{F}_{k-n}\hat{\phi}_n\right)^2\right]^{\frac{1}{2}}, \qquad \text{(A.20)}
\end{aligned}$$

where in the latter equality we have first replaced $\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}}$ in (A.19) with $\sum_{\varkappa=-\frac{N}{2}+1}^{0}$ (per the comment following Equation (A.9)) and then substituted $k-N$ for k. The expression in (A.20) is clearly bounded by a constant times the extended l^2 norm of Equation (A.8),

$$\|f(\cdot)\phi\|_{l^2_{ext}} \equiv \left[2\pi \sum_{k=-N+2}^{N} \left(\sum_{n\in I_{n,k}} \hat{F}_{k-n}\hat{\phi}_n\right)^2\right]^{\frac{1}{2}}, \qquad \text{(A.21)}$$

for which:

$$\|f(\cdot)\phi\|_{l^2_{ext}} \leq \|f\|_\infty \|\phi\|_{l^2_{ext}} = \|f\|_\infty \|\phi\|_{l^2}, \qquad \text{(A.22)}$$

(where $\|\phi\|_{l^2_{ext}}$ is defined by zero padding).

Hence, in Equation (A.15) (and similarly in Equation (A.16)), the sum over $k \in \varkappa_1$ is bounded by $c\|\phi\|_{l^2}$.

The sum over $k \in \varkappa_2$ (see Equation (A.18)) requires different estimate. For example, consider Equation (A.15). For $k \in \varkappa_2$, we have:

$$k + N - n \geq \frac{N}{4} \text{ when } n \in \left[-\frac{N}{2}+1, \frac{N}{2}\right]. \qquad \text{(A.23)}$$

Moreover, $\hat{f}_k$ (the Fourier coefficients of f) decay like $O(k^{-s})$, where s is the number of continuous derivatives of f, and it is easily seen that when $s > 1$, $\hat{F}_k$ also decays like $O(k^{-s})$.

Hence,

$$|\hat{F}_{k+N-n}| \leq c|k+N-n|^{-s} \leq c\Big(\frac{N}{4}\Big)^{-s}, \tag{A.24}$$

per Equation (A.23). It follows that the sum over $k \in \varkappa_2$ satisfies the bound:

$$\begin{aligned}
&\left[2\pi \sum_{k\in\varkappa_2}\Big(\sum_{n\in J_{n,k}} \frac{N}{k}\hat{F}_{k+N-n}\hat{\phi}_n\Big)^2\right]^{\frac{1}{2}} \\
\leq & cN^{-s+1}\left[\sum_{|k|\leq\frac{N}{4}}\Big(\sum_{n\in J_{n,k}}\hat{\phi}_n\Big)^2\right]^{\frac{1}{2}} \\
\leq & cN^{-s+2}\left[\sum_{|k|\leq\frac{N}{4}}\sum_{n\in J_{n,k}}\hat{\phi}_n^2\right]^{\frac{1}{2}} \\
\leq & cN^{-s+\frac{5}{2}}\|\phi\|_{l^2}.
\end{aligned} \tag{A.25}$$

Here we have used Equation (A.24) in the first inequality,

$$\Big(\sum_n \phi_n\Big)^2 \leq N^2 \sum_n \phi_n^2 \tag{A.26}$$

in the second, and replaced $\sum_{|k|\leq\frac{N}{4}}$ by $\frac{N}{4}$ in the third. It follows that when $s \geq \frac{5}{2}$, the sum over $k \in \varkappa_2$ in Equation (A.15) is bounded by $c\|\phi\|_{l^2}$. The sum over $k \in \varkappa_2$ in Equation (A.16) is bounded similarly. Thus, both Equation (A.15) and Equation (A.16) are bounded by $c\|\phi\|_{l^2}$, which finishes our estimate for the two sums in Equation (A.14). This completes the derivation of Equation (8.52).

Equation (8.53) readily follows by nothing that both $D_h S_h^{-1}(f(\cdot)\phi)_i$ and $S_h^{-1}(f(\cdot)S_h\phi)_i$ are $A_0(\phi)$ operators. The latter is a consequence of Equation (8.52) and the estimate

$$\begin{aligned}
\|S_h^{-1}(f(\cdot)\phi)_i\|_{l^2} &= \Big(\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} \frac{\widehat{(f\phi)}_k^{\,2}}{|k|^2} \Big)^{\frac{1}{2}} \\
&\leq \Big(\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} \widehat{(f\phi)}_k^{\,2} \Big)^{\frac{1}{2}} \\
&= \|f\phi\|_{l^2} \\
&\leq \|f\|_\infty \|\phi\|_{l^2}, \qquad \text{(A.27)}
\end{aligned}$$

where $\widehat{(f\phi)}_k$ is given by Equation (A.13). □

APPENDIX B

ESTIMATES FOR THE NONLINEAR TERMS IN THE VELOCITY VARIATION

We estimate the nonlinear terms (Equations (9.6), (9.9) and (9.11)) in the velocity variation. Consider first the expression Equation (9.6) for $\dot{U}_1^{NL}$. We expand some of the variations in this expression using Lemmas 8.0.11 and 8.0.12, for example,

$$\begin{aligned}\left(\frac{S_h\zeta_j}{\zeta_j-\tau_i}\right)^{\cdot} = &-\frac{\zeta_\alpha(\alpha_j)}{(\zeta(\alpha_j)-\tau(\alpha_i))^2}\big(\dot{\zeta}_j-\dot{\tau}_i\big)+\frac{S_h\dot{\zeta}_j}{\zeta(\alpha_j)-\tau(\alpha_i)}\\ &+\frac{\zeta_\alpha(\alpha_j)(\dot{\zeta}_j-\dot{\tau}_i)^2}{(\zeta(\alpha_j)-\tau(\alpha_i))^2(\zeta(\alpha_j)-\tau(\alpha_i)+\dot{\zeta}_j-\dot{\tau}_i)}\\ &+\mathrm{O}(h^s).\end{aligned} \tag{B.1}$$

To estimate the terms involving differences in (B.1), we make use of the Fourier series representation

$$\frac{\dot{\zeta}_j-\dot{\tau}_i}{\alpha_j-\alpha_i}=\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}}\hat{\dot{\zeta}}_k\frac{e^{ik\alpha_j}-e^{ik\alpha_i}}{\alpha_j-\alpha_i}, \tag{B.2}$$

so that

$$\begin{aligned}\left\|\frac{\dot{\zeta}_j-\dot{\tau}_i}{\alpha_j-\alpha_i}\right\|_{l^2}^2 &\le \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}}|\hat{\dot{\zeta}}_k|^2\left|\frac{e^{ik\alpha_j}-e^{ik\alpha_i}}{\alpha_j-\alpha_i}\right|^2\\ &\le \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}}|\hat{\dot{\zeta}}_k|^2k^2\\ &=\|S_h\dot{\zeta}\|_{l^2}^2.\end{aligned} \tag{B.3}$$

The first term on the right hand side of (B.1) is estimated by multiplying and dividing by $\big(\alpha_j-\alpha_i\big)^2$, and using (B.3) to obtain,

$$\left\|\frac{\zeta_\alpha(\alpha_j)(\dot{\zeta}_j-\dot{\tau}_i)}{(\zeta(\alpha_j)-\tau(\alpha_i))^2}\right\|_{l^2}\le\frac{c}{h}\|S_h\dot{\zeta}\|_{l^2}, \tag{B.4}$$

The extra factor $\frac{1}{h}$ comes from an extra factor of $\frac{1}{\alpha_j - \alpha_i}$. It is easy to see that the second term in Equation (B.1) is also bounded by $\frac{c}{h}\|S_h\dot{\zeta}\|_{l^2}$, and the third term is similarly bounded by $\frac{c}{h}\|S_h\dot{\zeta}\|_{l^2}^2$.

Returning the expression for $\dot{U}_1^{NL}$ in Equation (9.6), it follows from Equation (B.4) that the first sum of the right hand side of Equation (9.6) is bounded by

$$\frac{c}{h}\|\dot{\omega}\|_\infty\|S_h\dot{\zeta}\|_{l^2} + \mathrm{O}(h^s) \leq c\big(\|\dot{\theta}\|_{l^2} + \|\dot{\sigma}\|_{l^2}\big) + \mathrm{O}(h^s), \tag{B.5}$$

where the latter inequality is a consequence of Equation (8.43), and the fact that $\|\dot{\omega}\|_\infty \leq ch$, which in turn readily follows from Equation (9.74) and the assumptions (Equation (8.4)). The second sum on the right hand side of Equation (9.6) is similarly bounded by $c\big(\|\dot{\theta}\|_{l^2} + \|\dot{\sigma}\|_{l^2}\big) + \mathrm{O}(h^s)$. For the third term on the right hand side of Equation (9.6), we multiply and divide by $(\alpha_j - \alpha_i)^3$ inside the summation and use the estimate

$$\begin{aligned} \left\|\frac{(\dot{\zeta}_j - \dot{\tau}_i)^2}{(\alpha_j - \alpha_i)^3}\right\|_{l^2} &\leq \frac{c}{h}\|S_h\dot{\zeta}\|_{l^2}^2, \\ &\leq ch^{\frac{5}{2}}\|S_h\dot{\zeta}\|_{l^2}, \\ &\leq ch^{\frac{5}{2}}\big(\|\dot{\theta}\|_{l^2}^2 + \|\dot{\sigma}\|_{l^2}^2\big) \end{aligned} \tag{B.6}$$

in view of $S_h\dot{\zeta} = \mathrm{O}(h^{\frac{7}{5}})$ (see Remark 8.0.17 and Equation (8.43)). Putting this estimates together, we have shown that

$$\dot{U}_1^{NL} = A_0(\dot{\theta}) + A_{-s}(\dot{\sigma}) + \mathrm{O}(h^s), \tag{B.7}$$

(using $\dot{\sigma} = A_{-s}(\dot{\sigma})$). Estimates for $\dot{U}_2^{NL}$ and $\dot{U}_3^{NL}$ are performed similarly to $\dot{U}_1^{NL}$, and verify that

$$\dot{u}^{NL} = A_0(\dot{\theta}) + A_{-s}(\dot{\sigma}) + \mathrm{O}(h^s). \tag{B.8}$$

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