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The main result of this paper is a proof of the existence of a solution generated by a method for the variational assimilation of observational data into the two–dimensional, incompressible Euler equations. The data are assumed to be given by linear (measurement) functionals acting on the space of functions representing vorticity. From a practical point of view, the data are considered to be sparse and available on a fixed space–time domain.

The objective of the variational assimilation is to obtain an estimate of the vorticity which minimizes a cost functional. The cost functional is the sum of a generalized mean squared error in the dynamics, a generalized mean squared error in the initial condition, and a weighted squared error in the misfit to the observed data. These generalized mean squared errors are computed over the fixed space–time domain containing the data. The estimate then provides a best (generalized) least squares fit between the model, the initial condition, and the data.

A necessary condition for the estimate of vorticity to minimize the cost functional is that it must satisfy the corresponding system of Euler–Lagrange equations, which consist of a nonlinear, coupled system of partial differential equations with an initial condition, a final condition, and boundary conditions. Construction of a solution to the Euler–Lagrange equations is possible provided they are linearized through an iterative scheme.

Analysis of one such scheme motivates a reformulation of the variational problem in terms of an iterated linearization of the dynamics. This second method results in a slightly different iterated system of Euler–Lagrange equations. The sequence of solutions generated is shown to be bounded in the Sobolev space $W^{k,p}$ (in space–time). It follows from a Sobolev imbedding theorem that the sequence contains a convergent subsequence, the limit of which is a classical solution of the nonlinear, forced Euler equation corresponding to the forward problem of the Euler–Lagrange system.

The two schemes mentioned above are compared based on formal applications of Newton's method to the operators defining the systems. We conclude that the two formulations of the assimilation problem are in fact different and provide some intuitive reasons for preferring the second method, beyond the fact that the existence proof is established.

Existence of a Solution to a Variational Data Assimilation Method in Two–dimensional Hydrodynamics

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Existence of a Solution to a Variational Data Assimilation Method in Two–dimensional Hydrodynamics

1. Introduction

Interest in improving numerical forecasting and hindcasting in meteorology and oceanography has led to the dedication of many resources to solving variational data assimilation problems. In the case of forecasting, the data to be assimilated are available at the initial time (and earlier) of the forecast period. The data are usually sparse in comparison with a model state and so an estimate of the initial state based on the available data becomes necessary. That is, the data do not provide a complete model initialization. In the case of a hindcast, the data to be assimilated are available over some fixed space–time domain, and sparse in both space and time. A hindcast consists of an estimate of the state over the entire space–time domain in which the data are available. Creating a hindcast over some time interval, say $[T_1, T_2]$, is one means for creating an initialization (at time T_2) for a forecasting model which is to begin at time T_2 (Bennett, *et al.*, 1992).

One specific approach to hindcasting is to find an estimate of the state which minimizes, over a fixed space–time domain, the sum of a generalized mean squared error in dynamics, a generalized mean squared error in the initial condition, and a generalized mean squared error between measurements of the estimated state and a set of observed data (Bennett, 1990; Bennett and Budgell, 1987; Bennett and Budgell, 1989; Bennett and Miller, 1991;

Bennett, *et al.*, 1992; Courtier and Talagrand, 1987; Foreman, *et al.*, 1992; Talagrand and Courtier, 1987). This formulation may be considered as a deterministic control problem where the forcing error and initial error are the control variables. As a prototype for the hindcast problem we study the application of this approach to the assimilation of data into the two-dimensional, incompressible Euler equations (in vorticity form). This has many of the mathematical features of the systems used in modeling atmospheric and oceanic dynamics, in particular, it has the difficult feature of being nonlinear.

We consider a model as consisting of a description of the dynamics (which is the vorticity equation) and a description of the means and covariances of the initial condition error, the dynamical error and the data error (section 3.1). The error covariances have the effect of setting the control parameters used in the forcing and initial conditions. When the "extra" information contained in the data and the error covariances are required to be used, the dynamical model as an operator is overdetermined. In general, the inversion of an overdetermined operator is called a *generalized inverse* (Reid, 1968). We accomplish a type of inversion by providing an estimate of vorticity corresponding to finding an extremum of a cost functional which consists of the generalized mean squared errors mentioned above (see section 3.2). In terms of control theory this requires providing estimates of the control variables. When the inverse method includes the errors mentioned it is referred to as a *weak constraint* formulation of the assimilation problem. In contrast, a *strong constraint* formulation excludes the dynamical error from the cost functional and may even exclude initial error as was the case in Courtier and Talagrand, 1987. This has been shown to lead to ill–conditioned inverse problems (Bennett and Miller, 1991).

An extremum of the cost functional does not *a priori* correspond to a solution which minimizes the cost functional. This is because the functional is not convex with respect to vorticity, due to the nonlinearity in the dynamics. The estimates of vorticity corresponding to extremals of the cost functional will be referred to as *smoothing solutions.* This name is motivated by the fact that we are attempting to find an estimate which is near the data (in terms of minimum cost) and weakly constrained by the dynamics (also in terms of minimum cost), providing a smoothed version of the data.

An extremum of the cost functional must satisfy the corresponding Euler–Lagrange (EL) system and solving this system is the way in which the smoothing solutions are found. The EL system resulting from the weak constraint problem for the two-dimensional Euler equation is a coupled non-linear system of partial differential equations with initial and final conditions (section 3.2). To solve the EL system an iterative scheme was proposed by Bennett and Thorburn (1992). The scheme is described in section 4.1 and in this paper is referred as the Generalized Inverse Method (GIM).

It is argued in section 6.2 that the sequence produced by GIM admits a linear instability. This provides a forcing feedback as iteration proceeds, and may prevent the sequence from being bounded. Inspection of the iterative scheme leads to a reformulation of the generalized inverse for which this mechanism is not present. The vorticity equation is first iterated in order to linearize the dynamics leading to a sequence of extremal problems. This second type of inverse has been demonstrated to be of practical interest (Bennett and Thorburn, 1992) and will be referred to in this paper as the Extended Kalman Smoother Method (EKSM) (see section 4.2). We establish the global existence of an EKSM solution over a finite space–time domain of arbitrary size. A prerequisite for establishing a generalized inverse by either the Generalized Inverse Method or the Extended Kalman Smoother Method is the global existence of a solution to the two-dimensional Euler equations. This has been established in various contexts by, for example, Wolibner (1933), Judovič (1966a), and Kato (1967).

Our proof of the global existence of an EKSM solution is motivated by the existence proofs for the two-dimensional Euler equations by Judovič (1966a) and the quasi–geostrophic equations by Bennett and Kloeden (1980). The EKSM consists of a sequence of linear partial differential equations whose solution generates a sequence of functions. The sequence of solutions is shown to be bounded in the Sobolev space $W^{k,p}$ (in space–time), where $p > 2$ and $k \geq 2$, with differentiability conditions on the covariances and the initial iterate. An appropriate choice of k and p allows the Sobolev imbedding of $W^{k,p}$ into a space of continuous functions, implying there exists a convergent subsequence whose limit has the necessary continuity to satisfy the forward problem of the nonlinear Euler–Lagrange equations in the classical sense.

2. Some Mathematical Preliminaries

2.1 Notation

Let $\Omega \subset R^2$ be an open, bounded, simply-connected region. We require Ω to have a locally Lipschitz boundary, $\partial\Omega$. That is, for every point $x \in \partial\Omega$, there exists a neighborhood of x, U_x, such that $\partial\Omega \cap U_x$ is the graph of a Lipschitz function. A Lipschitz function is continuous, possibly with corners, but the corners can not be cusps. Of particular interest is the case where Ω is a rectangular region, since this is typical of the domains used in fluid models such as local–area oceanic and atmospheric models.

Let $T > 0$ be a fixed real number, and $S = \Omega \times (0, T)$. The closure of S, $\overline{S} = \Omega \cup \partial\Omega \times [0, T]$, is the space–time domain over which we wish to obtain a smoothing function. We will be considering two types of functions defined on S, scalar functions having values in $\mathbb{R}^1$, and vector functions having values in $\mathbb{R}^2$, each with $t \in [0, T]$ considered as a parameter. For a scalar function $\phi = \phi(x, t)$, where $x = (x_1, x_2) \in \Omega$, $\nabla\phi = (\phi_{x_1}, \phi_{x_2})$ is the usual (spatial) two-dimensional gradient operator, where subscripts denote partial differentiation. It will be convenient to use the notation $\nabla^{\perp}\phi$ for the vector $(-\phi_{x_2}, \phi_{x_1})$ perpendicular (with a particular orientation) to the gradient. The Laplacian of ϕ will be denoted $\Delta\phi = \phi_{x_1x_1} + \phi_{x_2x_2}$. Each of these operators may be applied for any value of t in $[0, T]$.

By a vector, v, in $\mathbb{R}^n$ we will mean an $n \times 1$ matrix, which has a $1 \times n$ matrix transpose, $v^* = [v_1, \ldots, v_n]$. Similarly, for any matrix M, we denote its transpose by M^*.

2.2 Function spaces and imbedding theorems

We separate the regularity in time from that of regularity in space where it is convenient and therefore use suitable notation involving, S or Ω, to distinguish between these situations. For general remarks we use $\mathcal{D}$ to represent either the entire space–time domain S, or the space domain Ω. The closure of $\mathcal{D}$ is $\overline{\mathcal{D}} = \mathcal{D} \cup \partial\mathcal{D}$. Thus, if $\mathcal{D}$ represents Ω, then $\overline{\mathcal{D}} = \overline{\Omega}$. If $\mathcal{D}$ represents S, then $\overline{\mathcal{D}} = \overline{\Omega} \times [0, T]$.

We utilize the Sobolev spaces of p-integrable functions on $\mathcal{D}$ which have k weak derivatives which are also p-integrable. That is, $W^{k,p}(\mathcal{D}) = \{f \in L^p(\mathcal{D}) : D^\beta f \in L^p(\mathcal{D}) \text{ for } 0 \leq |\beta| \leq k\}$, where we use the multi-index notation for derivatives. Hence, $D^\beta = D_{x_1}^{\beta_1} D_{x_2}^{\beta_2} D_t^{\beta_3}$, where $D_t^{\beta_3}$ is excluded when $\mathcal{D}$ represents Ω. Also, the order of the derivative corresponds to the order of the multi-index, given by $|\beta| = \beta_1 + \cdots + \beta_n$, $n = 2$, or $n = 3$. For $\|\cdot\|_{p,\mathcal{D}} = \|\cdot\|_{0,p,\mathcal{D}}$ denoting the $L^p(\mathcal{D})$-norm, the functional $\|\cdot\|_{k,p,\mathcal{D}}$ defined by

$$\|f\|_{k,p,\mathcal{D}} = \left[\sum_{0 \leq |\beta| \leq m} \|D^\beta f\|_{p,\mathcal{D}}^p \right]^{1/p} \qquad \text{if } 1 \leq p < \infty \;, \tag{2.2.1}$$

defines a norm on $W^{k,p}(\mathcal{D})$. For a function $f(x,t)$ defined on S, we mean by $\|f\|_{k,p,\Omega}$ that the norm is applied to the spatial coordinates x, with t considered as a parameter.

Extensive coverage of the properties of Sobolev spaces may be found in (Adams, 1975). We state some theorems and properties which are used in this application and refer the interested reader to Adams' book (Adams, 1975) for further details.

The main result of this paper relies on the following property of imbeddings. The space of functions $W^{k,p}(\mathcal{D})$ is a space of equivalence classes of $L^p(\mathcal{D})$-functions, two members of a class being equivalent if they differ only on a set of Lebesgue measure zero. When $W^{k,p}(\mathcal{D})$ is *imbedded* in $C^j(\overline{\mathcal{D}})$, for an appropriate j, each equivalence class in $W^{k,p}(\mathcal{D})$ contains an element of $C^j(\overline{\mathcal{D}})$. The space $C^j(\overline{\mathcal{D}})$ is the space of functions which have up to j^{th}–order uniformly continuous derivatives on $\mathcal{D}$ with continuous extensions to the boundary. Consequently, with no loss of generality, we may consider the elements of $W^{k,p}$ as C^j functions. When $W^{k,p}(\mathcal{D})$ is *compactly imbedded* in $C^j(\overline{\mathcal{D}})$, any sequence bounded in $W^{k,p}(\mathcal{D})$ has a subsequence which converges in the C^j topology to a $C^j(\overline{\mathcal{D}})$-function. This is formally stated in the Rellich-Kondrachov imbedding theorem which is the refinement of the Sobolev imbedding theorem to compact imbeddings. We write it in the following fashion.

Theorem 2.2.1 *(theorem 6.2, part III* Adams, 1975*) If $\mathcal{D} \subset \mathbb{R}^n$ is bounded with a locally Lipschitz boundary, then the following imbedding is compact:*

$$W^{j+m,p}(\mathcal{D}) \;\rightarrow\; C^j(\overline{\mathcal{D}}) \qquad \textit{if } mp > n \; .$$

Thus, for example, $W^{3,3}(S)$ is compactly imbedded into $C^1(\overline{S})$ (for $m = 2$, $p = 3$, $\dim(S) = n = 3$), which means that any sequence, $\{u_n\}$, bounded in $W^{3,3}(S)$ has a subsequence which converges in the C^1 topology to a C^1-function. Furthermore, any function, u, in $W^{3,3}(S)$ is equal to a C^1-function, $\tilde{u}$, except on a set of measure zero. Hence, we may identify the maximum of $|D^1 u|$ with the maximum of $|D^1 \tilde{u}|$. Note further that any function in $W^{3,4}(S)$ is equivalent to a C^2–function. This "extra" order of differentiability (from C^1 to C^2) obtained by increasing the order of integrability (from $W^{3,3}$ to $W^{3,4}$) allows a needed elliptic estimate. The elliptic estimate bounds derivatives of velocities in terms of the natural logarithm of the norm of the vorticity in $W^{k,p}(\Omega)$ (see Lemma 5.1.4 and equation (5.1.14)).

Another fact which will be utilized throughout is that $W^{k,p}(\mathcal{D})$ is a Banach Algebra for $kp > n = \dim(\mathcal{D})$ (Adams, 1975). That is, for $f, g \in W^{k,p}(\mathcal{D})$,

$$\|fg\|_{k,p,\mathcal{D}} \leq c\|f\|_{k,p,\mathcal{D}}\|g\|_{k,p,\mathcal{D}} \, . \tag{2.2.2}$$

The constants appearing in various estimates will be denoted by a lower case "c", and subscripted if there is more than one in a given equation. The values of these constants may change from equation to equation.

3. Description of the Problem

3.1 The dynamical model

Consider the vorticity equation for the motion of a two-dimensional, incompressible fluid in the region Ω:

$$\begin{aligned} &\zeta_t + v(\zeta)\cdot\nabla\zeta = F(x,t) \quad \text{for} \quad (x,t)\in\Omega\times[0,T] \\ &v(\zeta)\cdot n = 0, \qquad \text{for} \quad x\in\partial\Omega,\ t\in[0,T] \\ &\zeta(x,0) = \zeta^0(x)\ , \end{aligned} \tag{3.1.1}$$

where n denotes the outward unit normal to Ω.

The (scalar) vorticity, ζ, is related to a stream function, ψ, through the boundary value problem

$$\begin{aligned} \Delta\psi(x,t) &= \zeta(x,t) \qquad \text{for } x\in\Omega \\ \psi(x,t) &= 0 \qquad \text{for } x\in\partial\Omega\ , \end{aligned} \tag{3.1.2}$$

at each time $t\in[0,T]$. The unique solution to (3.1.2) may be written $\psi = G\zeta$ where G is the integral operator defined by the Green's function, $g(x,y)$, for the Dirichlet problem in Ω. That is, let $g(x,y)$ be the Green's function for Ω, and G the integral operator defined by

$$G\zeta(x,t) = \int_\Omega g(x,y)\,\zeta(y,t)\,dy\ , \tag{3.1.3}$$

where t may be considered as a parameter. Then $\psi = G\zeta$ is the solution (for a given t) of (3.1.2).

The velocity, $v(\zeta)$, is the divergence free vector field given by $\nabla^\perp(G\zeta) = (-(G\zeta)_y, (G\zeta)_x)$. This is given formally by $k\times\nabla(G\zeta)$, where k is normal to the two dimensional plane of fluid motion. Note that v is well defined as an operator since the first (weak) derivatives of $G\zeta$ exist (see Lemma 5.1.2 and Lemma 5.3.2).

The boundary condition in equation (3.1.1) may be generalized to include Lipschitz domains by instead requiring that $G\zeta(x,t) = 0$ for all points $x \in \partial\Omega$, for all $t \in [0,T]$. This ensures that the normal velocity is zero when an outward normal is defined, and allows "corners" since the boundary condition is well defined at any such corners.

Now suppose that we are using this model in an effort to predict the behavior of a particular "real" fluid. Then $F(x,t)$ represents a first guess to the forcing in the system (perhaps based on some observations of the forcing) and this will inherently not be known perfectly. To allow for this uncertainty we include an additional term in the model as part of the forcing term, representing the error in the first guess. Similarly, we allow for error in the initial condition since this will involve some observation as well. That is, we modify the model to be

$$
\begin{aligned}
\zeta_t + v(\zeta)\cdot\nabla\zeta = F(x,t) + q(x,t) \quad &\text{for} \quad (x,t) \in \Omega\times[0,T] \\
G\zeta(x,t) = 0, \qquad &\text{for} \quad x \in \partial\Omega,\ t\in[0,T] \\
\zeta(x,0) = \zeta^0(x) + a(x) \quad &\text{for } x \in \Omega\ .
\end{aligned}
\tag{3.1.4}
$$

where $F(x,t)$ and $\zeta^0(x)$ are first estimates of the source of vorticity in Ω and the initial vorticity, while $q(x,t)$ and $a(x)$ are functions representing the error in the first estimates. Indeed, by specifying two functions

$$
Q : (\Omega\times[0,T])\times(\Omega\times[0,T]) \mapsto \mathbb{R}^1 \qquad \text{and} \qquad A : \Omega\times\Omega \mapsto \mathbb{R}^1\ , \tag{3.1.5}
$$

each symmetric and positive definite on its domain, there exist zero mean random variables q and a such that

$$
E(q(x,t)q(x',t')) = Q(x,t,x',t') \qquad \text{and} \qquad E(a(x)a(x')) = A(x,x')\ , \tag{3.1.6}
$$

where E represents the expectation while Q and A are in fact the auto-covariance functions corresponding to the random variables (Cramèr and Leadbetter, 1967). However, we will consider the functions q and a to be deterministic control variables. In which case Q and A may be considered to be the kernels of (covariance) operators formally related to weighting factors in the cost functional defined below (equations (3.2.3–4). These kernels implicitly affect the allowable range of controls to be applied. In practice, *estimates* for Q and A are made from various analyses of data where prior knowledge of what factors contribute to the errors is available (Bennett, *et al.*, 1992).

Note that while we are introducing control variables in the forcing and initial conditions in equation (3.1.4), we are not doing so with the boundary conditions or the condition $div\, v(\zeta) = 0$. Hence, the rigid boundary condition and the relation between vorticity and stream function, $\Delta\psi = \zeta$, are strong constraints. As a consequence, the relation of vorticity to velocity, $v(\zeta) = \nabla^{\perp} G\zeta$, remains a strong constraint as well.

We will say that a function ζ is a *first guess solution* if it solves (3.1.1). That is, a first guess solution satisfies the dynamical equations when no forcing error, $q(x,t)$, and initial error, $a(x)$, are present. Note that since (3.1.1) is nonlinear, the solution of (3.1.4) is not the sum of a first guess solution and a solution of (3.1.1) with $q(x,t)$ as the forcing and $a(x)$ as the initial condition.

We consider a finite set of data d^k, for $k = 1, 2, \ldots, M$, consisting of a sampling of the vorticity given by linear functionals $\mathcal{L}^k : \zeta \mapsto R$, plus a sampling error ϵ^k. That is,

$$d^k = \mathcal{L}^k(\zeta(x,t)) + \epsilon^k \ . \tag{3.1.7}$$

For notational convenience we may write this as an M-vector,

$$d = \mathcal{L}(\zeta) + \epsilon \ . \tag{3.1.8}$$

The auto-covariance of ϵ^k is assumed to be known and will be the $(M \times M)$-matrix w^{-1}. We again consider w^{-1} to be formally related to w which is a weight factor in a cost functional. The linear functionals $\mathcal{L}^k$ could, for example, be evaluation of ζ at the point (x_k, t_k) which may be represented as integration against a kernel distribution,

$$\mathcal{L}^k(\zeta) = \int_0^T dt \int_\Omega dx \, \delta(x - x_k) \, \delta(t - t_k) \, \zeta(x,t) = \zeta(x_k, t_k) \ . \tag{3.1.9}$$

Alternatively, the kernel could have a smoothing property (that is, *not* point-wise evaluation) which more realistically represents the tendency of a physical sampling process to be spread over a small space-time domain. This may be expressed as

$$\mathcal{L}^k(\zeta) = \int_0^T dt \int_\Omega dx \, \mathcal{K}^k(x, t, x_k, t_k) G\zeta(x,t) \ , \tag{3.1.10}$$

where $\mathcal{K}^k$ is any smooth function with support in a neighborhood of (x_k, t_k). Other nonlocal forms of measurements such as empirical orthogonal functionals or line averaged quantities can be expressed in this form, in which case the measurement kernel is not localized. We note that in actual applications it is convenient to consider sampling the stream function rather than vorticity directly, thus we include the linear integral operator G as part of the measurement process.

3.2 The minimization problem and the Euler-Lagrange system

Let the functions $W(x,t,x',t')$ and $V(x,x')$, where

$$W : (\overline{\Omega} \times [0,T]) \times (\overline{\Omega} \times [0,T]) \mapsto \mathbb{R}^1 \qquad \text{and} \qquad V : \overline{\Omega} \times \overline{\Omega} \mapsto \mathbb{R}^1 \ , \tag{3.2.1}$$

be defined as the formal "functional inverses" of the covariances $Q(x,t,x',t')$ and $A(x,x')$ by satisfying the following properties (Bennett and Thorburn, 1992; Tarantola, 1987).

$$\begin{aligned} \int_0^T dt' \int_\Omega dx' Q(x,t,x',t') W(x',t',y,\tau) &= \delta(x-y)\delta(t-\tau) \\ \int_\Omega dx' A(x,x') V(x',y) &= \delta(x-y) \ . \end{aligned} \tag{3.2.2}$$

The functions $W(x,t,x',t')$ and $V(x,x')$ are the kernels of *weighting operators* in the sense of Tarantola, 1987.

The objective is to make an estimate of vorticity , $\hat{\zeta}$, so that the corresponding error in forcing, $\hat{q}$, error in the initial condition, $\hat{a}$, and error in the measurements, $\hat{\epsilon}$, are minimal over the fixed space–time domain in a weighted least-squares sense. Specifically, we wish to minimize the cost functional $\mathcal{J}(\zeta)$ over an appropriate class of functions $\mathcal{W}$, where

$$\begin{aligned} \mathcal{J}(\zeta) = & \int_0^T dt \int_\Omega dx \int_0^T dt' \int_\Omega dx' \ q(x,t) W(x,t,x',t') q(x',t') \\ & + \int_\Omega dx \int_\Omega dx' a(x) V(x,x') a(x') \\ & + \epsilon^* w \epsilon \ . \end{aligned} \tag{3.2.3}$$

The choice of an estimate $\hat{\zeta}$ which minimizes $\mathcal{J}$ will firstly smooth the data, in the sense that measurements of $\hat{\zeta}$ will be near the data. Secondly, the estimate $\hat{\zeta}$ will be interpretable as a vorticity, in the sense that it is constrained to satisfy the dynamics.

Rewriting the cost functional by formally replacing $q(x,t)$ with $\zeta_t + v(\zeta)\cdot\nabla\zeta - F$, $a(x)$ with $\zeta(x,0) - \zeta^0(x)$, and the vector notation for the matrix multiplication in the third term, we see the weighted least-squares form explicitly in terms of the errors in dynamics, initial conditions and measurements,

$$\begin{aligned}\mathcal{J}(\zeta) = \int_0^T dt \int_\Omega dx \int_0^T dt' \int_\Omega dx' \, (\zeta_t + v(\zeta)\cdot\nabla\zeta - F(x,t))W(x,t,x',t')\times \\ (\zeta_t + v(\zeta)\cdot\nabla\zeta - F(x',t')) + \\ \int_\Omega dx \int_\Omega dx' [\zeta(x,0) - \zeta^0(x)]V(x,x')[\zeta(x',0) - \zeta^0(x')] + \\ \sum_{k,l}[d^k - \mathcal{L}^k(\zeta)]w_{kl}[d^l - \mathcal{L}^l(\zeta)] \, .\end{aligned} \tag{3.2.4}$$

A necessary condition for $\mathcal{J}(\zeta)$ to be minimized by a particular choice $\zeta = \hat{\zeta}$ is that $\hat{\zeta}$ must be a local extremum for $\mathcal{J}(\zeta)$. The calculus of variations may be used to find the Euler-Lagrange (EL) system whose solution will be such an extremum (Gelfand and Fomin, 1963). That is, a necessary condition for ζ to be a local extremum of $\mathcal{J}(\zeta)$ is that ζ must satisfy the following Euler-Lagrange system.

$$\zeta_t + v(\zeta)\cdot\nabla\zeta = F(x,t) + Q \bullet \mu(x,t) \tag{3.2.5a}$$

$$\zeta(x,0) = \zeta^0(x) + A \circ \mu(x,0) \tag{3.2.5b}$$

$$-\mu_t - v(\zeta)\cdot\nabla\mu - G[\nabla^\perp\mu\cdot\nabla\zeta] = \tag{3.2.6a}$$

$$[\mathcal{L}_{(\xi,\tau)}(\delta(x-\xi)\delta(t-\tau))]^*\mathbf{w}[d - \mathcal{L}(\zeta)]$$

$$\mu(x,T) = 0 \tag{3.2.6b}$$

In equation (3.2.5a), $Q \bullet \mu$ is given by

$$(Q \bullet \mu)(x,t) = \int_0^T dt' \int_\Omega dx' Q(x,t,x',t')\mu(x',t') \, . \tag{3.2.7}$$

Similarly, $A \circ \mu$ in (3.2.5b) is given by

$$(A \circ \mu)(x, 0) = \int_{\Omega} dx' A(x, x')\mu(x', 0) \ . \tag{3.2.8}$$

The last term of (3.2.6a), $\mathcal{L}_{(\xi,\tau)}(\delta(x-\xi)\delta(t-\tau))$ indicates that the measurement functional, defined by (3.1.10), acts on the variables (ξ, τ). That is,

$$\mathcal{L}^k_{(\xi,\tau)}(\delta(x-\xi)\delta(t-\tau)) = \int_0^T d\tau \int_{\Omega} d\xi \, \mathcal{K}^k(\xi, \tau, x_k, t_k) \, G(\delta(x-\xi, t-\tau)) \ . \tag{3.2.9}$$

The adjoint variable, μ, is defined to be the weighted forcing error,

$$\mu(x, t) = \int_0^T d\tau \int_{\Omega} dy \ W(x, t, y, \tau) q(y, \tau) \ . \tag{3.2.10}$$

The derivation of the Euler-Lagrange system is outlined in Appendix A. Notice that (3.2.5 and 3.2.6) form a coupled nonlinear boundary value problem in time, with initial and final conditions. The adjoint equation (3.2.6) is forced by a weighted sum of delta functions with the weights depending on measuring vorticity. The equations are also coupled through the advective term $v(\zeta) \cdot \nabla\mu$ and the term $G[\nabla^{\perp}\mu \cdot \nabla\zeta]$ in the adjoint equation (3.2.6a). If we can somehow decouple the system through an iterative process, the adjoint equation (3.2.6) can be integrated "backwards", from T to 0. This would then determine a correction to the initial condition in (3.2.5b) and the forcing in (3.2.5a) so that integrating the "forward" equation will lead to a solution which passes within prescirbed error of the data.

Comparing (3.2.5) with (3.1.4) we see that $Q \bullet \mu$ is the estimate of the forcing control, q(x,t), and $A \circ \mu$ is the estimate of the initial control, a(x).

4. Solution of the Euler-Lagrange System

4.1 The Generalized Inverse Method (GIM)

A standard approach for proving existence of solutions and numerically approximating a solution to a nonlinear system such as (3.2.5–6) is to iterate the equations in such a way as to linearize about the previous iterate. In Chapter 6 a formal tangent linearization is developed in which Newton's method is applied to obtain an iteration scheme. This is compared to the results developed in the present chapter. For now we invoke a type of linearization by selecting terms in the equations and evaluating them as present (n^{th}–level) iterates or previous ($(n-1)^{\text{st}}$–level) iterates. There are several possible ways of selecting the terms, besides components of the nonlinear terms, which will be treated as previous ($(n-1)^{\text{st}}$–level) iterates. A particular choice for the system (3.2.6–7) is the following.

$$(\zeta_n)_t + v(\zeta_n)\cdot\nabla\zeta_n = F + Q \bullet \mu_{n-1} \tag{4.1.1a}$$

$$\zeta_n(x,0) = \zeta^0(x) + A \circ \mu_n(x,0) \tag{4.1.1b}$$

$$-(\mu_n)_t - v(\zeta_{n-1})\cdot\nabla\mu_n - G[\nabla^\perp\mu_n\cdot\nabla\zeta_{n-1}] = \\ [\mathcal{L}_{(\xi,\tau)}\,(\delta(x-\xi)\delta(t-\tau))]^* w[d - \mathcal{L}(\zeta_{n-1})] \tag{4.1.2a}$$

$$\mu_n(x,T) = 0\ . \tag{4.1.2b}$$

This choice is attractive in that the fewest fields have been evaluated at the $(n-1)^{\text{st}}$ level, and uniqueness may be established for μ_n using an energy argument, and for ζ_n using the results of Judovič (1966a). However, since the adjoint equation for μ_n (equation (4.1.2)) is not a simple integral along characteristics, there is no obvious way to generate a solution. Furthermore, the term $G[\nabla^\perp\mu_n\cdot\nabla\zeta_{n-1}]$ admits a linear instability which may prevent a bound on the growth of μ_n as iteration proceeds, even over the fixed time interval $[0, T]$. The interpretation of this term as a "growth" term is discussed in more detail in chapter 6. This has lead the authors in Bennett, *et al.*, 1992 and Bennett and Thorburn, 1992 to adopt the following scheme.

$$(\zeta_n)_t + v(\zeta_{n-1}) \cdot \nabla\zeta_n = F + Q \bullet \mu_n \tag{4.1.3a}$$

$$\zeta_n(x, 0) = \zeta^0(x) + A \circ \mu_n(x, 0) \tag{4.1.3b}$$

$$-(\mu_n)_t - v(\zeta_{n-1}) \cdot \nabla\mu_n - G[\nabla^\perp\mu_{n-1} \cdot \nabla\zeta_{n-1}] = \tag{4.1.4a}$$

$$[\mathcal{L}_{(\xi,\tau)}\,(\delta(x-\xi)\delta(t-\tau))]^* w[d - \mathcal{L}(\zeta_n)]$$

$$\mu_n(x, T) = 0 \ . \tag{4.1.4b}$$

Assuming that ζ_{n-1} and μ_{n-1} are known, define the linear operator L_n by

$$L_n(\eta) = \eta_t + v(\zeta_{n-1}) \cdot \nabla\eta \ . \tag{4.1.5}$$

That is, L_n represents the derivative along a path determined by the velocity field from the previous ($(n-1)^{\text{st}}$–level) iterate.

Also, let J_{n-1} be the third term in (4.1.4a), that is,

$$J_{n-1} = G[\nabla^\perp\mu_{n-1} \cdot \nabla\zeta_{n-1}] \ . \tag{4.1.6}$$

Equations (4.1.3–4) become

$$L_n(\zeta_n) = F + Q \bullet \mu_n \tag{4.1.9a}$$

$$\zeta_n(x, 0) = \zeta^0(x) + A \circ \mu_n(x, 0) \tag{4.1.9b}$$

$$-L_n(\mu_n) = J_{n-1} + \tag{4.1.10a}$$

$$[\mathcal{L}_{(\xi,\tau)}(\,\delta(x-\xi)\delta(t-\tau))]^* w[d - \mathcal{L}(\zeta_n)]$$

$$\mu_n(x, T) = 0 \ . \tag{4.1.10b}$$

For each $n \geq 1$, (4.1.9–10) form an inhomogeneous coupled linear system for ζ_n and μ_n. The uniqueness of solutions for the coupled system (4.1.9–10) is slightly involved and is shown in Appendix B. The approach is the same as in Bennett and Miller (1991), where the authors have established uniqueness for a linear single-level quasi-geostrophic model whose domain is a rectangle, with periodic boundary conditions.

The solutions generated by solving equations (4.1.9–10) form a sequence whose limit, if it exists, is the result of having produced a generalized inverse to the operator determined by the model dynamics, the data, and the statistics of the data and model errors. We will refer to the iterative solution method given by (4.1.9–10) (equivalently, (4.1.3–4)) as the Generalized Inverse Method (GIM).

4.2 The Extended Kalman Smoother Method (EKSM)

The term J_{n-1} in equation (4.1.10a) arises from formally allowing independent functional variations of the advecting velocity, $v(\zeta)$, when computing the first variation of the cost functional (3.2.4). A simplification can be made by assuming that the advecting velocities are *not* allowed a functional variation. That is, the cost functional is defined in terms of the linearized dynamics by fixing the advecting velocity in (3.1.4). Once an estimate for the vorticity is obtained by solving the EL system, a new advecting velocity may be defined from the estimate. This leads to another cost functional based on the latest estimate of velocity. The sequence of cost functionals may be written as

$$\mathcal{J}^n(\zeta_n) = \int_0^T dt' \int_\Omega dx' \; (L_n(\zeta_n(x,t)) - F)W(x,t,x',t')(L_n(\zeta_n(x',t')) - F)$$
$$+ \int_\Omega dx \int_\Omega dx' [\zeta_n(x,0) - \zeta^0(x)]V(x,x')[\zeta_n(x',0) - \zeta^0(x')]$$
$$+ \sum_{k,l} [d^k - \mathcal{L}^k(\zeta_n)]w_{kl}[d^l - \mathcal{L}^l(\zeta_n)] \; . \tag{4.2.1}$$

The EL system corresponding to a stationary solution of (4.2.1) is the following system.

$$L_n(\zeta_n) = F + Q \bullet \mu_n \tag{4.2.2a}$$

$$\zeta_n(x,0) = \zeta^0(x) + A \circ \mu_n(x,0) \tag{4.2.2b}$$

$$-L_n(\mu_n) = \tag{4.2.3a}$$

$$[\mathcal{L}_{(\xi,\tau)}(\,\delta(x-\xi)\delta(t-\tau))]^* w[d - \mathcal{L}(\zeta_n)]$$

$$\mu_n(x,T) = 0 \; . \tag{4.2.3b}$$

Uniqueness of solutions to equations (4.2.2–3) is shown in Appendix B. The solutions to the system (4.2.2–3) form a sequence each member of which is the result of having formed a generalized inverse to the operator determined by the linear model dynamics (dependent on the given element of the sequence), the data, and the statistics of the errors in the linear model and the data. If the limit of the sequence exists, it is intuitive that it will be different from the limit found using GIM since the equations differ by the term J_{n-1}. That is, equations (4.2.2–3) are the same as (4.1.9–10) with $J_{n-1} \equiv 0$ and, in the limit as n tends to infinity, converge to different systems of nonlinear partial differential equations. To distinguish these approaches for finding a generalized inverse we call the iterative solution method given by (4.2.2–3) the Extended Kalman Smoother Method (EKSM). The notion that the GIM and EKSM may lead to different types of generalized inverse solutions is explored further in Chapter 6.

The name 'Extended Kalman Smoother' was chosen by Bennett and Thorburn (1992) to suggest the similarity to the extended Kalman filter (Gelb, 1974). The present approach, as well as that of Bennett and Thorburn (1992), is formally deterministic and the name is only intended as an analogy.

4.3 Construction of solutions

To construct a solution to the system (4.1.9–10), define M scalar *representer functions* $r_n^1,\ldots,r_n^M$, or in vector form $r_n = (r_n^1,\ldots,r_n^M)^*$, and their adjoints $\alpha_n = (\alpha_n^1,\ldots,\alpha_n^M)^*$ by

$$L_n(r_n) = Q \bullet \alpha_n \qquad (4.3.1a)$$

$$r_n(x,0) = A \circ \alpha_n(x,0) \qquad (4.3.1b)$$

$$-L_n(\alpha_n) = \qquad (4.3.2a)$$

$$[\mathcal{L}_{(\xi,\tau)}(\,\delta(x-\xi)\delta(t-\tau))]$$

$$\alpha_n(x,T) = 0\;. \qquad (4.3.2b)$$

Application of L_n, $Q\bullet$, and $A\circ$ to vectors is meant component-wise. A solution to the system (4.3.1–2) may be constructed by first finding α_n as the solution to the final value problem (4.3.2). Once this is known r_n may be obtained by solving the initial value problem (4.3.1). A proof that solutions to the system (4.3.1–2) are unique follows the same argument as given in Appendix B for the systems (4.1.9–10) and (4.2.2–3).

In Appendix C it is shown that the action of the measurement functionals, $\mathcal{L}^j(\cdot)$, may be expressed as an inner product with the representer functions, $\langle r_n^j,\cdot\rangle$, for each iteration n. That is, $\mathcal{L}^j(\cdot) = \langle r_n^j,\cdot\rangle$ (equation C2).

The Riesz representation theorem asserts the uniqueness of this relation, meaning that there is only one function r_n^j which represents the action of the measurement functional $\mathcal{L}^j$. Hence, the functions r_n are appropriately named "representer functions".

Next, denote the n^{th} first guess solution by ζ_{F_n} and μ_{F_n}. That is, ζ_{F_n} and μ_{F_n} are solutions to the following system.

$$L_n(\zeta_{F_n}) = F + Q \bullet \mu_{F_n} \tag{4.3.3a}$$

$$\zeta_{F_n}(x,0) = \zeta^0(x) + A \circ \mu_{F_n}(x,0) \tag{4.3.3b}$$

$$L_n(\mu_{F_n}) = J_{n-1} \tag{4.3.4a}$$

$$\mu_{F_n}(x,T) = 0 \tag{4.3.4b}$$

Now consider the sum of the n^{th} first guess solutions and a linear combination of the representers. That is, let

$$\zeta_n(x,t) = \zeta_{F_n}(x,t) + b_n^* r_n(x,t) \tag{4.3.5a}$$

$$\mu_n(x,t) = \mu_{F_n}(x,t) + b_n^* \alpha_n(x,t) \ , \tag{4.3.5b}$$

where $b_n^* = (b_n^1, \ldots, b_n^M)$.

We may derive an algebraic system of equations which has solution b_n by substituting the expansion (4.3.5) into the system (4.1.9–10), using the equations defining the representers (4.3.1–2) and the first–guess (4.3.3–4), and equating coefficients of $\mathcal{L}_{(\xi,\tau)}(\delta(x-\xi)\delta(t-\tau))$. The matrix system has the form

$$P_n b_n = h_n \tag{4.3.6}$$

where

$$h_n = d - \mathcal{L}_{(\xi,\tau)}(\zeta_{F_n}) \quad \text{and} \tag{4.3.7}$$

$$P_n = R_n + w^{-1} \ . \tag{4.3.8}$$

Recall that the iteration index is n and in the above equations P_n, R_n and w^{-1} are M by M matrices while b_n, h_n, d and $\mathcal{L}_{\xi,\tau}(\zeta_{F_n})$ are vectors in $\mathbb{R}^M$. In the last equation, (4.3.8), R_n is the $M \times M$ matrix of representers where the $(i,j)^{\text{th}}$ element is given by the j^{th} measurement functional, $\mathcal{L}^j$ applied to the i^{th} representer, r_n^i,

$$(R_n)_{ij} = \mathcal{L}^j(r_n^i)\ . \tag{4.3.9}$$

We will show that R_n is a symmetric, positive definite matrix in Lemma 4.3.1 and Lemma 4.3.2 which follow. Thus, P_n is also a symmetric, positive definite matrix and invertible for each n. From the matrix equation (4.3.6) we obtain the sequence of representer coefficients

$$b_n = P_n^{-1} h_n\ . \tag{4.3.10}$$

Lemma 4.3.1 *The matrix of measured representers, R_n, is symmetric.*

Proof: We first define the fundamental solution (or influence function), $\Gamma(x,t,y,\tau)$, for the equations governing the representers (4.3.1–2). The fundamental solution depends on the iterate, n, but we are concerned with only a fixed iterate and so do not indicate this dependence with a subscript. The symmetry of the fundamental solution will be apparent. Then a simple calculation shows that the representer matrix R_n is obtained by applying the measurement functional to each of the dependencies (x,t) and (y,τ) in the fundamental solution Γ. This solution being symmetric with respect to interchange of (x,t) and (y,τ) implies the symmetry of R_n.

Let $\{\Gamma(x,t,y,\tau), \gamma(x,t,y,\tau)\}$ be functions which satisfy the following system.

$$L_n\Gamma = \int_0^T dt' \int_\Omega dx' Q(x,t,x',t')\gamma(x',t',y,\tau) \tag{4.3.11a}$$

$$\Gamma(x,0,y,\tau) = \int_\Omega dx' A(x,x')\gamma(x,0,y,\tau) \tag{4.3.11b}$$

$$-L_n\gamma = \delta(x-y,t-\tau) \tag{4.3.12a}$$

$$\gamma(x,T,y,\tau) = 0 \ , \tag{4.3.12b}$$

where $L_n = \partial/\partial t + v(\zeta_{n-1}) \cdot \nabla$, as in (4.1.5). The solution Γ may be expressed as an integral involving the influence function γ, as shown by the following construction. The subscript on the differential operator L_n will be suppressed, and instead replaced by notation to specify on which variables it is to act. Thus $L_{(\xi,\eta)} = \partial/\partial\eta + v(\zeta_{n-1}) \cdot \nabla_\xi$ specifies the spatial derivative in ξ and the time derivative in η.

Applying the weight operator W to the equation governing Γ (4.3.11a),

$$\int_0^T dt' \int_\Omega dx' W(x,t,x',t') L_{(x',t')}\Gamma(x',t',y,\tau) = \tag{4.3.13}$$

$$\int_0^T dt' \int_\Omega dx' W(x,t,x',t') \int_0^T dt'' \int_\Omega dx'' Q(x',t',x'',t'')\gamma(x'',t'',y,\tau)$$

$$= \int_0^T dt'' \int_\Omega dx'' \delta(x-x'',t-t'')\gamma(x'',t'',y,\tau)$$

$$= \gamma(x,t,y,\tau) \ .$$

Now apply the differential operator $L_{(x,t)}$ to each side of equation the above equation (4.3.13). The result is

$$\int_0^T dt' \int_\Omega dx' \{ -L_{(x,t)} W(x,t,x',t') L_{(x',t')}\Gamma(x',t',y,\tau)\} = \tag{4.3.14}$$

$$-L_{(x,t)}\gamma(x,t,y,\tau) = \delta(x-y,t-\tau) \ .$$

If we multiply each side of equation (4.3.14) by $\Gamma(x,t,\xi,\eta)$ and integrate over the (x,t) domain we have

$$\Gamma(y,\tau,\xi,\eta) = \tag{4.3.15}$$
$$\int_0^T dt \int_\Omega dx \int_0^T dt' \int_\Omega dx' \Gamma(x,t,\xi,\eta)\{-L_{(x,t)}W(x,t,x',t')L_{(x',t')}\Gamma(x',t',y,\tau)\} \ .$$

Using the relation given in (4.3.13) to rewrite the last term in (4.3.15) we have

$$\Gamma(y,\tau,\xi,\eta) = \tag{4.3.16}$$
$$\int_0^T dt \int_\Omega dx \Gamma(x,t,\xi,\eta)\{-L_{(x,t)}\gamma(x,t,y,\tau)\} \ .$$

Integrating by parts and using the equation for Γ (4.3.11), we obtain an integral representation for Γ in terms of γ,

$$\Gamma(y,\tau,\xi,\eta) = \tag{4.3.17}$$
$$\int_0^T dt \int_\Omega dx \int_0^T dt' \int_\Omega dx' \gamma(x,t,y,\tau)Q(x,t,x',t')\gamma(x',t',\xi,\eta)$$
$$+ \int_\Omega dx \int_\Omega dx' \gamma(x,0,y,\tau)A(x,x')\gamma(x',0,\xi,\eta) \ .$$

Note that, by inspection of the integrals in (4.3.17), Γ is symmetric in the sense that

$$\Gamma(y,\tau,\xi,\eta) = \Gamma(\xi,\eta,y,\tau) \ , \tag{4.3.18}$$

provided that Q and A are symmetric.

From Γ we are able to construct the representer matrix by applying the measurement functional to each of the pairs of independent variables in $\Gamma(y,\tau,\xi,\eta)$. That is, we will show that the representer matrix defined in (4.3.9) is given by

$$R_{ij} = \mathcal{L}^j_{(x,t)}\mathcal{L}^i_{(y,\tau)}\Gamma(x,t,y,\tau) \ . \tag{4.3.19}$$

To prove the relationship given by (4.3.19), first apply the measurement functional $\mathcal{L}^j_{(y,\tau)}$ to the equation governing γ (4.3.12) to obtain

$$-L_{(x,t)}\mathcal{L}^j_{(y,\tau)}\gamma(x,t,y,\tau) = \mathcal{L}^j_{(y,\tau)}(\delta(x-y,t-\tau) \qquad (4.3.20)$$
$$\mathcal{L}^j_{(y,\tau)}\gamma(x,T,y,\tau) = 0 \ .$$

By uniqueness of solutions to the adjoint representer equation (4.3.2), we must have the relation

$$\mathcal{L}^j_{(y,\tau)}\gamma(x,t,y,\tau) = \alpha^j(x,t) \ . \qquad (4.3.21)$$

Applying $\mathcal{L}^j_{(y,\tau)}$ to the equation for Γ (4.3.11) and substituting α_j for $\mathcal{L}^j_{(y,\tau)}\gamma$ we have

$$L_{(x,t)}\mathcal{L}^j_{(y,\tau)}\Gamma(x,t,y,\tau) = Q \bullet \alpha^j(x,t) \qquad (4.3.22a)$$
$$L_{(x,t)}\mathcal{L}^j_{(y,\tau)}\Gamma(x,0,y,\tau) = A \circ \alpha^j(x,0) \ . \qquad (4.3.22b)$$

Using the fact that solutions to the representer equations (4.3.1) are unique, we have the relation

$$\mathcal{L}^j_{(y,\tau)}\Gamma(x,t,y,\tau) = r^j(x,t) \ . \qquad (4.3.23)$$

By applying the measurement functional to the representers r^j we obtain

$$R_{ij} = \mathcal{L}^j_{(x,t)}\big(r_i(x,t)\big) \qquad (4.3.24)$$
$$= \mathcal{L}^j_{(x,t)}\mathcal{L}^i_{(y,\tau)}\Gamma(x,t,y,\tau) \ .$$

The symmetry of Γ with respect to (x,t) and (y,τ) given by (4.3.18) implies the symmetry with respect to i and j of R_{ij} in (4.3.24). This concludes the proof of Lemma 4.3.1

Lemma 4.3.2 *The symmetric matrix of measured representers, R_n, is positive definite.*

Proof: Let $c \in \mathbb{R}^M$ be an arbitrary nonzero vector. Then, using the expression for R given by (4.3.24),

$$c^* R_n c = \sum_{i,j} c_j \mathcal{L}^j_{y,\tau} \mathcal{L}^i_{x,t} \Gamma(x,t,y,\tau) c_i \ . \tag{4.3.25}$$

Now replacing Γ in (4.3.25) by its expression in terms of γ using equation (4.3.17),

$$\begin{aligned} c^* R_n c = \\ \sum_{i,j} c_j \big[\mathcal{L}^j_{y,\tau} \mathcal{L}^i_{x,t} \int_0^T dt'' \int_\Omega dx'' \int_0^T dt' \int_\Omega dx' \gamma(x'',t'',x,t) Q(x'',t'',x',t') \times \\ \gamma(x',t',y,\tau) + \\ \int_\Omega dx'' \int_\Omega dx' \gamma(x'',0,x,t) A(x'',x') \gamma(x',0,y,\tau)\big] c_i \ . \end{aligned} \tag{4.3.26}$$

$$\begin{aligned} = \int_0^T dt'' \int_\Omega dx'' \int_0^T dt' \int_\Omega dx' \big[\sum_i c_i \mathcal{L}^i_{x,t} \gamma(x'',t'',x,t)\big] Q(x'',t'',x',t') \times \\ \big[\sum_j c_j \mathcal{L}^j_{y,\tau} \gamma(x',t',y,\tau)\big] + \\ \int_\Omega dx'' \int_\Omega dx' \big[\sum_i c_i \mathcal{L}^i_{x,t} \gamma(x'',0,x,t)\big] A(x'',x') \times \\ \big[\sum_j c_j \mathcal{L}^j_{y,\tau} \gamma(x',0,y,\tau)\big] \ . \end{aligned} \tag{4.3.27}$$

We rewrite equation (4.3.27) as

$$\begin{aligned} c^* R_n c = \\ = \int_0^T dt'' \int_\Omega dx'' \int_0^T dt' \int_\Omega dx' P_1(x'',t'') Q(x'',t'',x',t') P_1(x',t') + \\ \int_\Omega dx'' \int_\Omega dx' P_1(x'',0) A(x'',x') P_1(x',0) \ , \end{aligned} \tag{4.3.28}$$

where

$$P_1(\xi,\eta) = \sum_i c_i \mathcal{L}^i_{x,t}\gamma(\xi,\eta,x,t) \ . \tag{4.3.29}$$

By assumption, Q and A are positive definite so that $c^* R_n c$ in (4.3.28) will be positive if P_1 is nonzero for any $(x,t) \in S$ and for any $x \in \Omega$ at $t = 0$. Note that P_1 is just a linear combination of the adjoint representers (see equation (4.3.21)). That is,

$$P_1(\xi,\eta) = \sum_i c_i \mathcal{L}^i_{x,t}\alpha^i_n(\xi,\eta) \tag{4.3.30}$$

Since the adjoint representers are solutions to the linear equation (4.3.2), a linear combination of the adjoint representers must satisfy the equation

$$\begin{aligned} -L_n(P_1(x,t)) &= \sum_i c_i \mathcal{L}^i_{\xi,\tau}(\delta(x-\xi,t-\tau)) \\ P_1(x,T) &= 0 \ . \end{aligned} \tag{4.3.31}$$

By assumption, the measurement functionals are independent. That is, any linear combination of measurements of delta distributions, such as the right hand side of (4.3.31), is not zero whenever any c_i is not zero. Thus, even though $P_1(x,T) = 0$, $P_1(x,t)$ is nonzero for some $(x,t) \in S$ and for some $x \in \Omega$ at $t = 0$ due to the nonzero forcing in (4.3.31). This concludes the proof of Lemma 4.3.2.

The functions given by the sum of the first–guess solutions and the linear combination of representers defined by equation (4.3.5) are solutions to (4.1.9–4.1.10) provided that the coefficients b_n exist. The existence of b_n is guaranteed by the invertibility of P_n, given by (4.3.8), and the existence of the first–guess misfits h_n, given by (4.3.7). The h_n exist and are unique since ζ_{F_n} is uniquely determined by (4.3.3–4). By using the representer functions defined by (4.3.1—2) we are able to construct a solution to (4.1.9–10) in the form of the linear combination (4.3.5). The independence of the measurement functionals and the uniqueness of solutions to the representer equations (4.3.1–2) guarantees that the representers are linearly independent functions. The solution procedure developed in this section is a method suitable to numerical approximation, since it provides an explicit method for solving the original system (4.1.9–10) (Bennett and Thorburn, 1992; Bennett, *et al.*, 1992).

5. Global Existence of an EKSM Solution

5.1 a priori bounds

We would like establish the existence of a solution to the nonlinear EL system (3.2.5–6) by showing that the sequence given by (4.3.5) is bounded in an appropriate Sobolev space. However, in Chapter 6 we give an informal argument as to why we believe that this will not be possible. It is the nature of the nonlinearity that produces this difficulty. Therefore, for practical interest, we address the question of existence of an EKSM solution, that is, a solution to the system (4.2.2–3). The EKSM solution is currently being used in the context of ocean and atmosphere quasi–geostrophic models (Bennett, *et al.*, 1992; Bennett and Thorburn, 1992).

We establish the existence of a solution to the EKSM problem using equations (4.2.2–3) for an arbitrary smoother interval $[0, T]$. This is shown in the sense that there exists (at least) one convergent subsequence of the sequence of solutions to the system (4.2.2–3).

The existence of the solution to the elliptic equation (3.1.2) and its regularity properties may be found, for example, in Gilbarg and Trudinger (1983). This is summarized in the following lemma, which is Corollary 1 (equation (4.24)) of Judovič (1966b), except that we modify the statement of the boundary smoothness.

Lemma 5.1.1 *For ζ_n in $W^{k,p}(\Omega)$, $k \geq 0$ and $p > 2$, where Ω has a locally Lipschitz boundary, the unique solution ψ_n of (3.1.2) is in $W^{k+2,p}(\Omega)$, with*

$$\|\psi_n\|_{k+2,p,\Omega} \leq cp\|\zeta_n\|_{k,p,\Omega} ,$$

uniformly in $[0, T]$.

Proof: An examination of the proof by Judovič (1966b) reveals that the case of a locally Lipschitz boundary is easily accommodated. Interior local estimates of $D_{k+2}\psi_n$ follow by placing spheres inside Ω (lemma 3.2 Judovič, 1966b). Local boundary estimates are achieved by locally mapping neighborhoods of boundary points to hemispheres and applying lemma 3.4 of Judovič (1966b). Boundary corners may be locally mapped to quarter spheres, which reduce to estimates on hemispheres by even extensions of ψ_n. A locally Lipschitz domain may be covered by finitely many regions for which these local estimates hold. This process eventually leads to the global bound (see theorem 1 and corollary 1 of Judovič, 1966b). The basis of the proof is the Calderon–Zygmund inequality (Adams, 1975, Gilbarg and Trudinger, 1983) and the Sobolev imbedding theorem (Adams, 1975).

As a consequence of Lemma 5.1.1 we obtain the following estimate on the norm of velocity. This is an minor modification of lemma 1.4 of Judovič (1966a).

Lemma 5.1.2 *Given ζ_n in $W^{k,p}(\Omega)$, $k \geq 0$ and $p > 2$, there is a unique $v_n = v(\zeta_n)$ such that v_n is in $W^{k+1,p}(\Omega)$ and satisfies the bound*

$$\|v_n\|_{k+1,p,\Omega} \leq c\|\zeta_n\|_{k,p,\Omega} \ ,$$

uniformly in $[0, T]$.

Proof: We simply note that $\|v_n\|_{k+1,p,\Omega} = \|\nabla^{\perp}\psi_n\|_{k,p,\Omega} = \|(-(\psi_n)_y, (\psi_n)_x)\|_{k+1,p,\Omega} \leq \|\psi_n\|_{k+2,p,\Omega}$ and apply Lemma 5.1.1. Note that by Theorem 2.2.1, $W^{2,3} \times W^{1,2}[0,T]$ compactly imbeds into $C^1(\overline{\Omega}) \times C^0[0,T]$, thus if we are given $\zeta_n \in W^{1,3}(\Omega) \times W^{1,2}[0,T]$, we have $v_n \in W^{2,3}(\Omega) \times W^{1,2}[0,T]$ and v_n is equivalent to a $C^1(\overline{\Omega}) \times C^0[0,T]$-function.

Let $v : \overline{\Omega} \times [0,T] \mapsto \mathbb{R}^2$ be a $C^1(\overline{\Omega}) \times C^0([0,T])$ vector field, with $div\, v = 0$ in Ω and $v \cdot n = 0$ on $\partial\Omega$ (n being the outward normal to Ω). Let

$\gamma = \gamma(x,t,s)$ be the solution to the o.d.e.

$$\frac{d\gamma}{ds} = v(\gamma(s),s) \qquad (5.1.1)$$
$$\gamma(t) = x \ .$$

That is, $\gamma(x,t,s)$ is the position of the fluid particle at time s which passes through the point x at time t. The next lemma establishes the existence of the characteristics γ.

Lemma 5.1.3 (lemma 2.2 and lemma 2.3 (Kato, 1967)) *There exists a unique global solution $\gamma = \gamma(x,t,s)$ to problem (5.1.1) for $0 \le s \le T$ for any initial condition $\gamma(t) = x$ where $t \in [0,T]$ and $x \in \Omega$. Furthermore, the solution of (5.1.1) is C^1 in all three variables. For fixed t and s, the map $\Phi_{t,s} : \overline{\Omega} \mapsto \overline{\Omega}$ defined by $x \mapsto \gamma(x,t,s)$ is one-to-one and measure preserving, where $\partial\Omega \mapsto \partial\Omega$. The map $\Phi_{t,t}$ given by $x \mapsto \gamma(x,t,t)$ is the identity (i.e. $\gamma(x,t,t) \equiv x$) and $\Phi_{s,t}$ is defined as $\Phi_{t,s}^{-1}$.*

We will need to solve the following two types of problems. Given v as above, $\omega^0(x) \in C^0(\overline{\Omega})$, $\omega^T(x) \in C^0(\overline{\Omega})$, and $F \in C^0(\overline{\Omega}) \times C^0([0,T])$, find the solution to the initial-value problem

$$L\omega = \omega_t + v \cdot \nabla\omega = F(x,t) \qquad (5.1.2)$$
$$\omega(x,0) = \omega^0(x) \ ,$$

and the final-value problem

$$L\omega = \omega_t + v \cdot \nabla\omega = F(x,t) \qquad (5.1.3)$$
$$\omega(x,T) = \omega^T(x) \ .$$

Each of these may be solved by integrating the equation along a characteristic given by the solution to (5.1.1), $\gamma(x,t,s)$, for $0 \le s \le t$ or $t \le s \le T$, respectively. The solution to the initial-value problem (5.1.2) may then be expressed as

$$\omega(x,t) = \omega^0(\gamma(x,t,0)) + \int_0^t F(\gamma(x,t,s),s)\,ds \ . \qquad (5.1.4)$$

Similarly, the solution to the final-value problem (5.1.3) may be expressed as

$$\omega(x,t) = \omega^T(\gamma(x,t,T)) - \int_t^T F(\gamma(x,t,s),s)\, ds \; . \tag{5.1.5}$$

The preceding lemmas serve to establish the solvability of the linearized equations for the GIM (4.1.9–10), the representers (4.3.1–2), and the first-guess (4.3.3–4) for a given iterate n. We conclude this section with an estimate of the sequence of velocities, v_n, which follows from an elliptic estimate. The following lemma is an extension of lemma 1.5 of Judovič (1966a), where the second derivatives of the stream function are estimated in terms of the logarithm of the gradient of vorticity in $L_p(\Omega)$. (See also theorem 4.4 of Bennett and Kloeden (1980).)

Lemma 5.1.4 *Given ζ_n in $W^{k,p}(\Omega)$, $k \geq 1$ and $p > 2$, where $\partial\Omega$ is locally Lipschitz and* $\max_{x\in\Omega} |D^\beta \zeta_n| \leq M_k$ *for $|\beta| \leq k-1$ then $\psi_n = G\zeta_n$ satisfies the bound*

$$\max_{x\in\Omega} |D^\gamma \psi_n| \leq c_1 p \ln\{c_2 p + c_3 p \, \|\zeta\|_{k,p,\Omega}\} \; ,$$

where $|\gamma| \leq k+1$ and the c_i, $i = 1,2,3$, depend only on M_k.

Proof: First note that provided $p > 2$, $W^{k,p}(\Omega)$ compactly imbeds into $C^{k-1}(\overline{\Omega})$ (see section 2.2), so that assuming bounds on derivatives of ζ_n up to order $k-1$ is consistent. Such a bound is utilized below in equation (5.1.9). The proof of the theorem follows the proof by Judovič of lemma 1.5 (Judovič, 1966a) with the needed changes to accommodate the higher regularity.

Let $\eta = D^\gamma \psi_n$, where γ is an arbitrary multi-index with $|\gamma| \leq k+1$ and $\psi_n = G\zeta_n$. Using Sobolev's integral identity (Judovič, 1966a; Bennett and Kloeden, 1980; Adams, 1975) we have the relation

$$|\eta(x)|^m = \int_{V_0} \left[\xi_1(x)\, |\eta(y)|^m + m \frac{\eta(y)\, |\eta(y)|^{m-2}}{|x-y|} \xi_2(y) \cdot \nabla \eta(y) \right] dy \; , \tag{5.1.6}$$

where V_0 is an arbitrary fixed cone with vertex x contained in Ω, ξ_1 and $\xi_2 = (\xi_2^{(1)}, \xi_2^{(2)})$ are known functions, continuous and bounded on Ω.

Estimating the second term on the right using Hölder's (generalized) inequality we have

$$|\eta(x)|^m \le c_1 \|\eta\|_{m,\Omega}^m + c_2 m \|\nabla\eta\|_{p,\Omega} \|\eta\|_{(m-1)p_1,\Omega}^{m-1} , \qquad (5.1.7)$$

where c_2 depends on m and $p_1 = p(3p-2)/(p-1)(p-2)$.

Inequality (5.1.7) is then substituted into the power series expansion for $\exp(\delta|\eta|)$ where δ is an arbitrary real constant. That is,

$$\exp(\delta|\eta|) = 1 + \sum_{l=1}^{\infty} \frac{\delta^l |\eta|^l}{l!} \le$$
$$1 + c_1 \sum_{l=1}^{\infty} \frac{\delta^l}{l!} \|\eta\|_{l,\Omega}^l + \delta c_2 \|\nabla\eta\|_{p,\Omega} \sum_{l=1}^{\infty} \frac{\delta^{l-1}}{(l-1)!} \|\eta\|_{(l-1)p_1,\Omega}^{l-1} \qquad (5.1.8)$$

Lemma 5.1.1 is now used to estimate $\|\eta\|_{l,\Omega}$ by

$$\|\eta\|_{l,\Omega} = \|D^\gamma \psi_n\|_{l,\Omega} \le \|\psi_n\|_{k+1,l,\Omega} \le c_3 l \|\zeta_n\|_{k-1,l,\Omega} \le lM , \qquad (5.1.9)$$

where M is independent of l. Substituting the bound (5.1.9) into (5.1.8) we have

$$\exp(\delta|\eta|) \le$$
$$1 + c_1 \sum_{l=1}^{\infty} \frac{\delta^l}{l!} (lM)^l + \delta c_2 \|\nabla\eta\|_{p,\Omega} \sum_{l=1}^{\infty} \frac{\delta^{l-1}}{(l-1)!} (l-1)p_1 M)^{l-1} \qquad (5.1.10)$$

Stirling's formula for $l! = \sqrt{2\pi l}(l/e)^l(1 + 1/12l + \mathcal{O}(1/n^2))$ provides the bound $l^l/l! \le c_6 e^l$. Choosing $\delta < Mep_1$ the geometric series in (5.1.10) are convergent and produce the bound

$$e^{\delta|\eta|} \le c_7 + c_8 \|\nabla\eta\|_p . \qquad (5.1.11)$$

Finally, using Lemma 5.1.1 again to estimate $\|\nabla\eta\|_p$, and taking the logarithm of each side we have the desired result.

Lemma 5.1.4 allows us to establish a bound on the velocities, $v_n = v(\zeta_n)$, in $W^{k,p}(\Omega)$ as follows. Since,

$$\|v_n\|_{k,p}^p = \sum_{|\alpha|\le k} \|D^\alpha v_n\|_p^p = \sum_{|\alpha|\le k} \int_\Omega |D^\alpha v_n|^p \ , \tag{5.1.12}$$

and

$$\int_\Omega |D^\alpha v_n|^p \le \max_{x\in\Omega} |D^\alpha v_n||\Omega| \le |\Omega| \max_{x\in\Omega} |D^\beta \psi_n| \ , \tag{5.1.13}$$

where $|\beta| = |\alpha| + 1$, by applying Lemma 5.1.4 we obtain

$$\|v_n\|_{k,p}^p \le c_0|\Omega| \max_{x\in\Omega} |D^\beta \psi_n| \le |\Omega| c_1 \ln(c_2 + c_3\|\zeta_n\|_{k,p}) \ . \tag{5.1.14}$$

5.2 Regularity in space

For the EKSM solution we have $J_{n-1} = 0$ in the first–guess adjoint equation (4.3.4). Thus the first–guess adjoint equation is the final-value problem

$$\begin{aligned} -L_n(\mu_{F_n}) &= 0 \\ \mu_{F_n}(x,T) &= 0 \ . \end{aligned} \tag{5.2.1}$$

This is seen to be the same type of problem as given by (5.1.3), having the form

$$\begin{aligned} (\mu_{F_n})_t + v\cdot(\Delta\mu_{F_n}) &= 0 \\ \mu_{F_n}(x,T) &= 0 \ , \end{aligned} \tag{5.2.2}$$

where the vector field v is $v(\zeta_{n-1})$. Following (5.1.5), the solution is

$$\mu_{F_n}(x,t) = 0 \qquad \forall\,(x,t) \in \Omega \times [0,T] \ . \tag{5.2.3}$$

As a consequence of the first–guess adjoint being zero (equation (5.2.3)), the expansion (4.3.5) implies that the EKSM system (4.2.2–3) may be written as

$$L_n(\zeta_n) = F + Q \bullet b_n^* \alpha_n \tag{5.2.4a}$$

$$\zeta_n(x,0) = \zeta^0(x) + A \circ b_n^* \alpha_n(x,0) \ . \tag{5.2.4b}$$

$$-L_n(\alpha_n) = [\mathcal{L}_{(\xi,\tau)}(\delta(x-\xi)\delta(t-\tau))] \tag{5.2.5a}$$

$$\alpha_n(x,T) = 0 \ . \tag{5.2.5b}$$

While the system (5.2.4–5) would appear to have simplified the solution procedure developed in section 4.3, the presence of b_n in (4.2.4) still requires the complete methods of section 4.3. The system (5.2.4–5) merely represents a "rearrangement" of the constructive method.

We subsequently show that the sequence of coefficients, b_n, is bounded, the sequence of representer adjoints, α_n, is bounded, and this results in a bound on the sequence of vorticities, ζ_n.

From equation (5.2.3), the first–guess vorticity equation (4.3.3) reduces to

$$\begin{aligned} L_n(\zeta_{F_n}) &= F \\ \zeta(x,0) &= \zeta^0(x) \ . \end{aligned} \tag{5.2.6}$$

The solution may be written as in (5.1.4), that is,

$$\zeta_{F_n}(x,t) = \zeta^0(\gamma(x,t,0)) + \int_0^t F(\gamma(x,t,s),s)\,ds \ . \tag{5.2.7}$$

Consequently, the $L^2(S)$–norm of ζ_{F_n} is bounded independently of n,

$$\|\zeta_{F_n}\|_{2,S} \le \|\zeta^0\|_{2,S} + T\|F\|_{2,S} \ . \tag{5.2.8}$$

Lemma 5.2.1 $\|b_n\|_\infty = \max_{1\le j\le M} |b_n^j|$ *is bounded independently of* n.

Proof: From equation (4.3.10), we have

$$\|b_n\|_\infty = \|P_n^{-1} h_n\|_\infty \le \|P_n^{-1}\|_\infty \|h_n\|_\infty \, . \tag{5.2.9}$$

We establish the boundedness of each of the factors on the right hand side. Consider that

$$\begin{aligned} \|h_n\|_\infty &= \|d - \mathcal{L}[\zeta_{F_n}]\|_\infty \\ &\le \|d\|_\infty + \|\mathcal{L}[\zeta_{F_n}]\|_\infty \\ &\le c_1 + \max_{1\le i\le M} |\mathcal{L}^i(\zeta_{F_n})| \, . \end{aligned} \tag{5.2.10}$$

By assumption, the measurement functionals are bounded from $W^{k,p}(S)$ into $\mathbb{R}^1$ and so, using the bound (5.2.8) where the norm on $L^2(S) \cap W^{k,p}(S)$ is taken to be the $L^2(S)$-norm,

$$\begin{aligned} |\mathcal{L}^i(\zeta_{F_n})| &\le \|\mathcal{L}^i\|_{2,S} \|\zeta_{F_n}\|_{2,S} \\ &\le c_i(\|\zeta^0\|_{2,S} + T\|F\|_{2,S}) \, . \end{aligned} \tag{5.2.11}$$

Inequalities (5.2.10) and (5.2.11) imply that $\|h_n\|_\infty$ is bounded independently of n.

It remains to show that the matrix norm of P_n^{-1}, $\|P_n^{-1}\|_\infty$, is bounded independently of n. Since w and R_n are real and symmetric matrices, there exist orthogonal transformations Z_n and W such that

$$\begin{aligned} R_n &= Z_n^* \Lambda_n Z_n \, , \quad \text{and} \\ w &= W^* \omega W \, . \end{aligned} \tag{5.2.12}$$

In equation (5.2.12), $\Lambda_n = \operatorname{diag}[\lambda^1(R_n), \ldots, \lambda^M(R_n)]$ and $\omega = \operatorname{diag}[\lambda^1(w), \ldots, \lambda^M(w)]$ are diagonal matrices consisting of the eigenvalues of R_n, $\lambda^k(R_n)$, and the eigenvalues of w, $\lambda^k(w)$. Since R_n and w are positive definite we have

$$\begin{aligned} &0 < \lambda_n^1(R_n) \leq \lambda_n^2(R_n) \leq \ldots \leq \lambda_n^M(R_n) , \quad \text{and} \\ &0 < \lambda_n^1(w) \leq \lambda_n^2(w) \leq \ldots \leq \lambda_n^M(w) . \end{aligned} \tag{5.2.13}$$

Since P_n must be real, symmetric and positive definite, there exists an orthogonal transformation $\widetilde{Z}_n$ such that

$$P_n = \widetilde{Z}_n^* \text{diag}[\lambda^1(P_n), \ldots, \lambda^M(P_n)] \widetilde{Z}_n , \tag{5.2.14}$$

where $\lambda^k(P_n)$ is the k^{th} largest eigenvalue of P_n. Consequently,

$$P_n^{-1} = \widetilde{Z}_n \text{diag}[(\lambda^1(P_n))^{-1}, \ldots, (\lambda^M(P_n))^{-1}] \widetilde{Z}_n^* , \tag{5.2.15}$$

and since the matrix norm of $\widetilde{Z}_n$ and $\widetilde{Z}_n^*$ is unity,

$$\|P_n^{-1}\|_\infty \leq \max_{1 \leq k \leq M} \{(\lambda^k(P_n))^{-1}\} . \tag{5.2.16}$$

A result from linear algebra (see Wilkinson (1965), section 44) is the relation

$$\lambda^k(R_n) + \lambda^M(w^{-1}) \leq \lambda^k(R_n + w^{-1}) = \lambda^k(P_n) \leq \lambda^k(R_n) + \lambda^1(w^{-1}) , \tag{5.2.17}$$

from which we have the bound

$$\begin{aligned} (\lambda^k(P_n))^{-1} &= (\lambda^k(R_n + w^{-1}))^{-1} \\ &\leq (\lambda^k(R_n) + \lambda^1(w^{-1}))^{-1} \\ &\leq (\lambda^1(w^{-1}))^{-1} = \lambda^1(w) . \end{aligned} \tag{5.2.18}$$

Inequalities (5.2.16) and (5.2.18) establish a bound, independent of the iteration index n, on the norm of the matrix P_n^{-1}, concluding the proof of Lemma 5.2.1.

In the next lemma we establish bounds on the model forcing correction, $Q \bullet \alpha_n$, and initial condition correction, $A \circ \alpha_n$, by using the adjoint representer equation (4.3.2). Recall that $\mathcal{K}^j$ is the kernel of the measurement functional defined by (3.1.10) and appears in the measurement of delta functions in (4.3.2).

Lemma 5.2.2

a.) *For $\mathcal{K}^j \in C^0(\overline{S}) \times C^0(\overline{S})$, the sequence of solutions to the adjoint representer equation (4.3.2) is bounded in $L_p(\Omega)$, uniformly for $t \in [0,T]$.*

b.) *If $Q \in C^k(\overline{S}) \times C^k(\overline{S})$, $k \geq 0$, and $\alpha_n^j \in L_p(\Omega)$ uniformly in t, then $Q \bullet \alpha_n^j \in W^{k,p}(\Omega)$. If $A \in C^k(\overline{\Omega}) \times C^k(\overline{\Omega})$ and $\alpha_n^j(t=0) \in L_p(\Omega)$, then $A \circ \alpha_n^j \in W^{k,p}(\Omega)$.*

Proof: The j^{th} component of the representer adjoint equation (4.3.2) is the equation

$$-L_n(\alpha_n^j) = \mathcal{L}^j_{(\xi,\tau)}[\delta(x-\xi, t-\tau)] \qquad (5.2.19a)$$

$$\alpha_n^j(x,T) = 0 \; . \qquad (5.2.19b)$$

Multiplying by $p\alpha_n^j|\alpha_n^j|^{p-2}$, integrating over Ω, and using the condition that $div\,(v(\zeta_{n-1})) = 0$ yields the differential inequality

$$-\frac{\partial}{\partial t}\|\alpha_n^j\|_{p,\Omega} \leq \|\mathcal{L}^j_{(\xi,\tau)}[\delta(x-\xi,t-\tau)]\|_{p,\Omega} \; . \qquad (5.2.20)$$

Integrating with respect to t, for $t \in [0,T]$, we obtain

$$\|\alpha_n^j\|_{p,\Omega} \leq \int_o^T dt\, \|\mathcal{L}^j_{(\xi,\tau)}[\delta(x-\xi,t-\tau)]\|_{p,\Omega} \; . \qquad (5.2.21)$$

From (5.2.21), $\alpha_n^j \in L_p$ for all $t \in [0,T]$, provided the term on the right hand side of (5.2.21) is finite.

Consider the function $f(x,t)$ defined by

$$f(x,t) = \mathcal{L}^j_{(\xi,\tau)}[\delta(x-\xi,t-\tau)] \qquad (5.2.22)$$
$$= \int_0^T d\tau \int_\Omega d\xi \mathcal{K}^j(\xi,\tau,x_j,t_j) G[\delta(x-\xi,t-\tau)]$$
$$= \int_\Omega d\xi \mathcal{K}^j(\xi,t,x_j,t_j) N(x-\xi) \; .$$

We have used $N(x-\xi) = G[\delta(x-\xi)]$ to denote the fundamental solution of the Laplacian, that is, $N(x-\xi) = (2\pi)^{(-1)} \log|x-\xi|$.

Since $N(x-\xi)$ is in L_2 for Ω a bounded domain (which implies N is L_1) and $\mathcal{K}^j(\xi,t,x_j,t_j)$ is in $C^0(\overline{S})$ as a function of (ξ,t), we have that $f(x,t)$ is continuous on $\overline{\Omega} \times [0,T]$. It then follows that $f(x,t)$ is $L_p(\Omega) \times L_1[0,T]$. That is,

$$\int_0^T dt \|\mathcal{L}^j_{(\xi,\tau)}[\delta(x-\xi,t-\tau)]\|_{p,\Omega} = \int_0^T dt \|f(x,t)\|_{p,\Omega} < \infty \; . \qquad (5.2.23)$$

This establishes part (a) of the lemma.

It is possible to relax the assumption of continuity in ξ of $\mathcal{K}^j(\xi,t,x_j,t_j)$ to merely L_1 integrability. However, we consider a physical measurement process to be one which essentially is a smoothing operator, motivating the stronger assumption of continuity.

For part (b), we begin with the L^p norm of the β^{th} derivative ($|\beta| \le k$) of $Q \bullet \alpha^j_n$. That is,

$$\left\|D^\beta Q \bullet \alpha^j_n\right\|^p_{p,\Omega} = \int_\Omega dx \left| D^\beta \int_0^T dt' \int_\Omega dx' Q(x,t,x',t') \alpha^j_n(x',t') \right|^p$$
$$\le |\Omega| \max_{\substack{x\in\overline{\Omega} \\ (x',t')\in\overline{S}}} \left\{ \left| D^\beta Q(x,t,x',t') \right|^p \right\} \int_0^T dt' \int_\Omega dx' \left| \alpha^j_n(x',t') \right|^p$$
$$= |\Omega| \max_{\substack{x\in\overline{\Omega} \\ (x',t')\in\overline{S}}} \left\{ \left| D^\beta Q(x,t,x',t') \right|^p \right\} \int_I dt' \left\| \alpha^j_n \right\|^{p,\Omega}_p \qquad (5.2.24)$$

where $|\Omega| = \int_\Omega dx$. From the proof of part (a) we have a uniform bound on $\left\|\alpha_n^j\right\|_{p,\Omega}$, thus, the last integral in the inequality (5.2.24) is bounded. Summing over all β, $|\beta| \leq m$, we arrive at the needed bound.

The estimates for $\|A \circ \alpha_n^j(x,0)\|_{m,p,\Omega}$ are essentially the same calculation. From the β^{th} derivative of $A \circ \alpha_n^j(x,0)$,

$$\begin{aligned}
\|D^\beta A \circ \alpha_n^j\|_{p,\Omega}^p &= \int_\Omega dx \left| D^\beta \int_\Omega dx' \, A(x,x')\alpha_n^j(x',0) \right|^p \\
&\leq |\Omega| \max_{\substack{x\in\overline{\Omega} \\ x'\in\overline{\Omega}}} \left\{ \left|D^\beta A(x,x')\right|^p \right\} \int_\Omega dx' \left|\alpha_n^j(x',0)\right|^p \\
&\leq |\Omega| \max_{x\in\overline{\Omega}} \left\{ \left|D^\beta A(x,x')\right|^p \right\} \int_0^T dt \left\|\alpha_n^j\right\|_{p,\Omega}^p , \qquad (5.2.25)
\end{aligned}$$

which is bounded by a constant. Summing over β yields the bound on $A \circ \alpha_n$. This completes the proof of Lemma 5.2.2.

The next theorem establishes the spatial regularity of a solution to the EKSM by showing the existence of a convergent subsequence of the sequence given by (4.3.5a).

Theorem 5.2.3 *If $J_{n-1} = 0$ (in equation (4.3.4a)), $Q \in C^k(\overline{S}) \times C^k(\overline{S})$ and $A \in C^k(\overline{\Omega}) \times C^k(\overline{\Omega})$, then the sequence $\{\zeta_n\}$ defined by (4.3.5a) is bounded in $W^{k,p}(\Omega)$ with $\|\zeta_n\|_{k,p,\Omega} \in L_1[0,T]$, for $k \geq 1$ and $p > 2$, provided the initial iterate $\zeta_0(x,t)$ is in $W^{2,3}(S)$ and the forcing is in $W^{k,p}(\Omega)$ with $\|F\|_{k,p,\Omega} \in L_1[0,T]$.*

Proof: The strategy is based on that of Judovič (1966a), allowing for the required higher regularity of the forcing term introduced by the control variable, $Q \bullet b_n^* \alpha_n$, and the regularity of the initial control, $A \circ b_n * \alpha$. The problem as written in equation (5.2.4) appear to be an initial value problem. However, the inverse nature of the problem is still present in the computation of the vector b_n, which requires solving the representer equations. Fortunately we have a bound on the vector b_n in Lemma 5.2.1.

To construct the desired bound on ζ_n, take all the β^{th} derivatives, $|\beta| \leq k$, of (5.2.4)

$$(D^\beta \zeta_n)_t + \sum_{\alpha \leq \beta} \binom{\beta}{\alpha} D^\alpha v_{n-1} \cdot \nabla D^{\beta-\alpha} \zeta_n = D^\beta \mathcal{F}_n \;, \tag{5.2.26}$$

where $\mathcal{F}_n$ denotes $F + Q \bullet b_n^* \alpha_n$ and $v_{n-1} = v(\zeta_{n-1})$. For $\alpha = (\alpha_1, \alpha_2)$, the multi-index inequality $0 \leq \alpha \leq \beta$ means $0 \leq \alpha_i \leq \beta_i$ for $i = 1, 2$.

Multiplying (5.2.26) by $pD^\beta \zeta_n \left|D^\beta \zeta_n\right|^{p-2}$ and integrating over Ω we have

$$\begin{aligned} \frac{\partial}{\partial t} \left\|D^\beta \zeta_n\right\|_{p,\Omega}^p = &- \int_\Omega p \sum_{0 \leq \alpha \leq \beta} \binom{\beta}{\alpha} D^\alpha v_{n-1} \cdot \left(D^\beta \zeta_n \left|D^\beta \zeta_n\right|^{p-2} \nabla D^{\beta-\alpha} \zeta_n\right) \\ &+ p \int_\Omega D^\beta \zeta_n \left|D^\beta \zeta_n\right|^{p-2} D^\beta \mathcal{F}_n \;. \end{aligned} \tag{5.2.27}$$

In equation (5.2.27), the term in the sum for which $\alpha = 0$ has the form $\int_\Omega v_{n-1} \cdot \nabla |Z|^p$ where Z is $D^\beta \zeta_n$. This term will vanish since $div\,(v_{n-1}) = 0$ and $v_{n-1} \cdot n = 0$ on $\partial\Omega$. Consequently, the sum in (5.2.27) is over values of $\alpha \neq 0$, that is $0 < \alpha \leq \beta$.

Taking the absolute value of the right hand side of equation (5.2.27), the first term is bounded by

$$p \sum_{0 < \alpha \leq \beta} \binom{\beta}{\alpha} \int_\Omega |D^\alpha v_{n-1} \cdot D^{\beta-\alpha} \nabla \zeta_n| |D^\beta \zeta_n|^{p-1} \;. \tag{5.2.28}$$

Using Hölder's inequality we have

$$p \sum_{0 < \alpha \leq \beta} \binom{\beta}{\alpha} \|D^\alpha v_{n-1} \cdot D^{\beta-\alpha} \nabla \zeta_n\|_{0,p,\Omega} \|D^\beta \zeta_n\|_{0,p,\Omega}^{p-1} \;. \tag{5.2.29}$$

Writing the scalar product in component form, where $v_{n-1}^{i} = v^{i}(\zeta_{n-1})$ represents the i^{th} component of v_{n-1}, and

$$D^{(i,j)} = \frac{\partial^{i}}{\partial x_1^{i}} \frac{\partial^{j}}{\partial x_2^{j}} ,$$

we have the equivalent expression

$$p \sum_{0<\alpha\leq\beta} \binom{\beta}{\alpha} \left[\| D^{\alpha} v_{n-1}^{1} D^{\beta-\alpha+(1,0)} \zeta_n + D^{\alpha} v_{n-1}^{2} D^{\beta-\alpha+(0,1)} \zeta_n \|_{0,p,\Omega} \right] \times$$
$$\| D^{\beta} \zeta_n \|_{0,p,\Omega}^{p-1} , \qquad (5.2.30)$$

which is bounded by

$$p \sum_{0<\alpha\leq\beta} \binom{\beta}{\alpha} \left[\ \| D^{\alpha} v_{n-1}^{1} D^{\beta-\alpha+(1,0)} \zeta_n \|_{0,p,\Omega} + \| D^{\alpha} v_{n-1}^{2} D^{\beta-\alpha+(0,1)} \zeta_n \|_{0,p,\Omega} \right] \times$$
$$\| D^{\beta} \zeta_n \|_{0,p,\Omega}^{p-1}$$
$$\leq pc \left[\| v_{n-1}^{1} \zeta_n \|_{k,p,\Omega} + \| v_{n-1}^{2} \zeta_n \|_{k,p,\Omega} \right] \| D^{\beta} \zeta_n \|_{0,p,\Omega}^{p-1} . \qquad (5.2.31)$$

With the Banach Algebra property of $W^{k,p}(\Omega)$, $kp > 2$ (Adams, 1975; theorem 5.23) and bounds on the velocity components using $\| v_{n-1}^{i} \|_{k,p,\Omega} \leq \| v_{n-1} \|_{k,p,\Omega}$, the quantity in (5.2.31) is bounded by

$$pc_1 \| v_{n-1} \|_{k,p,\Omega} \| \zeta_n \|_{k,p,\Omega} \| D^{\beta} \zeta_n \|_{k,p,\Omega}^{p-1} . \qquad (5.2.32)$$

The right hand side of equation (5.2.27) can now be estimated using Hölder's inequality and the bound on the sum given by (5.2.32). This yields

$$\frac{\partial}{\partial t} \left\| D^{\beta} \zeta_n \right\|_{p,\Omega}^{p} \leq p \left\| D^{\beta} \zeta_n \right\|_{p,\Omega}^{p-1} \left\| D^{\beta} \mathcal{F}_n \right\|_{p,\Omega}$$
$$+ p 2^{k} \left\| v_{n-1} \right\|_{m,p} \left\| \zeta_n \right\|_{m,p} \left\| D^{\beta} \zeta_n \right\|_{p}^{p-1} , \qquad (5.2.33)$$

where 2^k bounds the constant $\sum \binom{\beta}{\alpha}$.

Using the bound on the velocity in equation (5.1.12), a consequence of Lemma 5.1.4, we can bound the norm of the velocity by $c_1 \ln\{pc_2 + pc_3\|\zeta_{n-1}\|_{k,p,\Omega}\}$, that is,

$$\frac{\partial}{\partial t}\|D^\beta \zeta_n\|_{p,\Omega}^p \le p\|D^\beta \zeta_n\|_{p,\Omega}^{p-1}\left\|D^\beta \mathcal{F}_n\right\|_{p,\Omega} + p2^k c_1 \ln\{pc_2 + pc_3\|\zeta_{n-1}\|_{k,p}\}\left\|\zeta_n\right\|_{k,p,\Omega}\left\|D^\beta \zeta_n\right\|_{p,\Omega}^{p-1} . \quad (5.2.34)$$

Summing on β, for $|\beta| \le k$,

$$\frac{\partial}{\partial t}\|\zeta_n\|_{k,p,\Omega}^p \le p\|\zeta_n\|_{k,p,\Omega}^{p-1}\left\|D^\beta \mathcal{F}_n\right\|_{p,\Omega} + p2^k c_1 \|\zeta_n\|_{k,p,\Omega}^p \ln\{pc_2 + pc_3\|\zeta_{n-1}\|_{k,p,\Omega}\} . \quad (5.2.35)$$

To simplify the notation, let $R_n(t) = \|\zeta_n\|_{k,p,\Omega}$ and $f_n = \|\mathcal{F}_n\|_{k,p,\Omega}$. This is in analogy to the notation introduced by Judovič (1966a). Then equation (5.2.35) is a differential inequality of the form

$$(R_n^p)_t \le pR_n^{p-1} f_n + pK_2 \ln(pc_2 + pc_3 R_{n-1}) R_n^p \quad (5.2.36a)$$

$$R_n(0) = \|\zeta_n(x,0)\|_{k,p,\Omega} = \|\zeta^0(x) + A \circ b_n^* \alpha_n(x,0)\|_{k,p,\Omega} , \quad (5.2.36b)$$

where $K_2 = c_1 2^k$. Equation (5.2.36) is analogous to equation 1.79 of Judovič (1966a).

Given a real constant $\delta > 0$, let $\overline{R}_n$ satisfy

$$(\overline{R}_n^p)_t \le p\overline{R}_n^{p-1} f_n + pc_5 \ln(pc_2 + pc_3 \overline{R}_{n-1}) \overline{R}_n^p \quad (5.2.37a)$$

$$\overline{R}_n(0) = R_n(0) + \delta . \quad (5.2.37b)$$

Since $R_n(0) \ge 0$ and $f_n \ge 0$, we then have $0 \le R_n \le \overline{R}_n$.

We can solve the differential inequality (5.2.37) formally by integrating each side of the equation with respect to t. This produces the relation

$$\overline{R}_n(t) \le R_n(0) + \delta + \int_0^t f_n(\tau)\,d\tau + \int_0^t c_5 \ln(pc_2 + pc_3\overline{R}_{n-1}(\tau))\overline{R}_n(\tau)\,d\tau . \quad (5.2.38)$$

Or, by defining $N_n = R_n(0) + \delta + \int_0^T f_n(\tau)d\tau$, we have

$$\overline{R}_n(t) \le N_n + \int_0^t c_5 \ln(pc_2 + pc_3\overline{R}_{n-1}(\tau))\overline{R}_n(\tau)\, d\tau \ , \tag{5.2.39}$$

corresponding to equation(1.82) of Judovič (1966a). Now multiply (5.2.39) by $c_5 \ln(pc_2 + pc_3\overline{R}_{n-1})\overline{R}_n$ and divide by $N_n + c_5 \int_0^T \ln(pc_2 + pc_3\overline{R}_{n-1})$ to observe that (5.2.38) can be written as

$$\frac{\partial}{\partial t} \ln\{N_n + c_5 \int_0^t \overline{R}_n \ln(pc_2 + pc_3\overline{R}_{n-1})\}\, d\tau \\ \le c_5 \ln(pc_2 + pc_3\overline{R}_{n-1}) \ . \tag{5.2.40}$$

This has the solution

$$N_n + c_5 \int_0^t \overline{R}_n \ln(pc_2 + pc_3\overline{R}_{n-1})\, d\tau \\ \le N_n \exp\{\int_0^t c_5 \ln(pc_2 + pc_3\overline{R}_{n-1})\, d\tau\} \ . \tag{5.2.41}$$

Combining the inequalities (5.2.39) and (5.2.41) we have

$$\overline{R}_n \le N_n \exp\{\int_0^t c_5 \ln(pc_2 + pc_3\overline{R}_{n-1})\, d\tau\} \ . \tag{5.2.42}$$

Multiplying each side of inequality (5.2.42) by pc_3, adding pc_2, and taking the logarithm we obtain

$$\gamma_n \le \ln(pc_2 + pc_3 N_n \exp\{\int_0^t c_5 \gamma_{n-1}\, d\tau\} \ , \tag{5.2.43}$$

where

$$\gamma_n = \ln(pc_2 + pc_3\overline{R}_n) \ . \tag{5.2.44}$$

Noting that for positive ξ,

$$\ln(a + be^{\xi}) \leq \xi + \ln(a + b) \ , \tag{5.2.45}$$

we obtain from (4.2.43) an inequality analogous to (1.91) of Judovič (1966a).

$$\gamma_n \leq \int_0^t c_5\gamma_{n-1} + \ln(pc_2 + pc_3 N_n) \ . \tag{5.2.46}$$

The last term in (5.2.46) can be shown to be independent of n in the following way. Looking back through the various substitutions we have

$$N_n = R_n(0) + \delta + \int_0^T f_n \tag{5.2.47}$$

$$= \|\zeta^0(x) + A \circ_n^* \alpha(x,0)\|_{k,p,\Omega} + \delta + \int_0^T \|F + Q \bullet b_n^* \alpha_n\|_{k,p,\Omega}$$

$$\leq \|\zeta^0(x)\|_{k,p,\Omega} + \int_0^T \|F\|_{k,p,\Omega} + \delta$$

$$+ \|A \circ \alpha_n^*(x,0)\|_{k,p,\Omega} + \int_0^T \|Q \bullet b_n^* \alpha_n\|_{k,p,\Omega} \ .$$

Consider the last two terms of (5.2.47). In particular, for $|\beta| \leq m$ we have

$$\|D^\beta Q \bullet b_n^* \alpha_n\|_{p,\Omega}^p = \int_\Omega dx \left| D^\beta \int_0^T dt' \int_\Omega dx' Q(x,t,x',t') b_n * \alpha(x',t') \right|^p$$

$$\leq \int_\Omega dx \sum_{j=1}^M |b_n^j|^p \left| \int_{\Omega_I} D^\beta Q \bullet \alpha_n^j \right|^p$$

$$\leq M \max_{1 \leq j \leq M} |b_n^j| \|D^\beta Q \bullet \alpha_n^j\|_p^p \ . \tag{5.2.48}$$

Summing on β we have

$$\|Q \bullet b_n^* \alpha_n\|_{k,p} \leq M \max_{1 \leq j \leq M} |b_n^j| \|Q \bullet \alpha_n^j\|_{k,p} \ . \tag{5.2.49}$$

Now inequality (5.2.47) shows that N_n is bounded independently of n. This follows since the first three terms, $\|\zeta^0(x)\|_{k,p,\Omega}+\int\limits_0^T \|F\|_{k,p,\Omega}+\delta$, are constants, and the last two terms, in view of the bound (5.2.49), Lemma 5.2.1, and Lemma 5.2.2, are bounded independently of n.

As a result of the bound on N_n, the last term in the inequality (5.2.46) is bounded independently of n, say by N_p. We therefore write equation (5.2.46) as

$$\gamma_n \leq \int\limits_0^t c_5\gamma_{n-1} + N_p \ . \tag{5.2.50}$$

Inequality (5.2.50) is precisely the same as inequality (2.40) of Judovič (1966a), allowing for differences in the definitions of γ_n and N_p. Hence, following the proof in Judovič, we obtain from induction the estimate

$$\gamma_n(t) \leq \frac{(c_5 t)^n}{n!}G_0 + (1 + c_5 t + \frac{(c_5 t)^2}{2!} + \cdots + \frac{(c_5 t)^{n-1}}{(n-1)!})N_p \ . \tag{5.2.51}$$

In inequality (5.2.51) G_0 is the maximum on $[0,T]$ of $\gamma_0(t)$, given by

$$\begin{aligned} G_0 &= \max_{t\in[0,T]} \gamma_0(t) = \max_{t\in[0,T]} \ln\{pc_2 + pc_3\overline{R}_0(t)\} \qquad (5.2.52) \\ &= \max_{t\in[0,T]} \ln\{pc_2 + pc_3(R_0(t)+\delta)\} \\ &= \max_{t\in[0,T]} \ln\{pc_2 + pc_3(\|\zeta_0(t)\|_{k,p,\Omega}+\delta)\} \ . \end{aligned}$$

We assume continuity of ζ_0, corresponding to a smooth initial iterate specified by ψ_0. It suffices to assume that $\zeta_0(x,t) \in W^{2,3}(S)$ since the compact embedding (Theorem 2.2.1) implies

$$W^{2,3}(S) \mapsto C^0(\overline{S}) \ .$$

That is, $\zeta_0(x,t)$ is equivalent to a $C^0(\overline{\Omega}) \times C^0[0,T]$–function. Therefore the maximum in (5.2.52), G_0, exists.

From inequality (5.2.51), we have the bound

$$\gamma_n(t) \le \frac{(c_5 T)^n}{n!} G_0 + N_p\, e^{c_5 T} . \tag{5.2.53}$$

In the limit as n tends to ∞, the first term on the right of inequality (5.2.53) tends to zero. We then have

$$\lim_{n\to\infty} \ln(pc_2 + pc_3 \overline{R}_n) \le N_p\, e^{c_5 T} , \tag{5.2.54}$$

from which it follows that

$$\lim_{n\to\infty} \overline{R}_n \le \quad c_6 \quad < \infty . \tag{5.2.55}$$

Finally, from (5.2.55) we have the desired bound on ζ_n. That is,

$$\begin{aligned} \lim_{n\to\infty} \|\zeta_n\|_{k,p,\Omega} = \lim_{n\to\infty} R_n \le \\ \lim_{n\to\infty} \overline{R}_n \le \quad c_6 \quad < \infty , \end{aligned} \tag{5.2.56}$$

where the constant, c_6, is independent of n and t. This concludes the proof of Theorem 5.2.3.

5.3 Regularity in time (existence)

In this section we establish a bound on the sequence $\{\zeta_n\}$, defined by equations (5.2.4–5), in the $W^{k,p}(S)$ norm, for $k \ge 1$ and $p > 2$. By the imbedding given in Theorem 2.2.1 we conclude that there is a convergent subsequence whose limit is a classical solution of (4.2.4) in the case $k \ge 2$ and $p > 3$, or $k \ge 3$ and $p \ge 3$.

We have relations between the spatial regularity of stream function, velocity, and vorticity from section 5.2. Combining these with the particular nature of equation (5.2.4) we extend various estimates of functions on Ω to functions on $S = \Omega \times [0, T]$. We begin with an extension of Lemma 5.1.1.

Lemma 5.3.1 *For ζ_n in $W^{k,p}(S)$, $k \geq 0$ and $p > 2$, where Ω has a locally Lipschitz boundary, the solution ψ_n of (3.1.2) is in $W^{k+2,p}(S)$, with*

$$\|\psi_n\|_{k+2,p,S} \leq cp\|\zeta_n\|_{k,p,S} \ ,$$

the bound being uniform on $[0, T]$.

Proof: Note that for $1 \leq m \leq k+2$, the elliptic problem $D_t^m \Delta\psi_n = D_t^m \zeta_n$ has solution $d_t^m \psi_n = G(D_t^m \zeta_n)$, and from Lemma 5.1.1 we have

$$\|D_t^m \psi_n\|_{k+2,p,\Omega} \leq \|D_t^m \zeta_n\|_{k,p,\Omega} \tag{5.3.1}$$

for all t in $[0, T]$. Thus,

$$\begin{aligned}
\|\psi_n\|_{k+2,p,S}^p &= \sum_{|\alpha| \leq k+2} \|D^\alpha \psi_n\|_{0,p,S}^p \\
&= \int_0^T dt\, \|\psi_n\|_{k+2,p,\Omega}^p + \sum_{m=1}^{k} \int_0^T dt\, \|D_t^m \psi_n\|_{k+2-m,p,\Omega}^p \\
&\leq \int_0^T dt\, c_1 \|\zeta_n\|_{k,p,\Omega}^p + \sum_{m=1}^{k} \int_0^T dt\, c_2 \|D_t^m \zeta_n\|_{k-m,p,\Omega}^p \\
&\leq c_3 \|\zeta_n\|_{k,p,S}^p + \sum_{m=1}^{k} c_4 \|\zeta_n\|_{k,p,S}^p \\
&\leq c_5 \|\zeta_n\|_{k,p,S}^p \ ,
\end{aligned} \tag{5.3.2}$$

which establishes the lemma.

A similar extension of Lemma 5.1.2 produces the following.

Lemma 5.3.2 *For $n \geq 0$ fixed, $\zeta_n \in W^{k,p}(S)$, $k \geq 0$ and $p > 2$, implies the bound on velocity*

$$\|v_n\|_{k+1,p,S} \leq c\|\zeta_n\|_{k,p,S} \ ,$$

the bound being uniform on $[0, T]$.

Proof: Simply note that $\|v_n\|_{k+1,p,S} = \|\nabla^{\perp}\psi_n\|_{k+1,p,S} \leq \|\psi_n\|_{k+2,p,S}$. Now apply Lemma 5.3.1.

Note that for $\zeta_n \in W^{1,4}(S)$ or $W^{2,3}(S)$, Lemma 5.3.2 implies $v_n \in W^{2,4}(S)$ or $W^{3,3}(S)$. By the imbedding theorem, Theorem 2.2.1, v_n is equivalent to a $C^1(\overline{S})$–function. The existence of the characteristics as solutions of (5.1.1) is then ensured by Lemma 5.1.3.

With the estimates given in Lemma 5.3.1 and Lemma 5.3.2 we are in a position to establish the following theorem, from which the existence result will follow.

Theorem 5.3.3 *Suppose the sequence* ζ_n *satisfies the hypothesis of Theorem 5.2.3 with the restriction that* $k \geq 2$. *Then* $\zeta_n \in W^{k,p}(S)$ $(k \geq 2$ *and* $p > 2)$ *and the sequence is bounded independently of* n *in* $W^{k,p}(S)$.

Proof: The proof is by induction on k. That is, assume that the sequence $\{\zeta_n\}$ is bounded in $W^{k,p}(\Omega)$ for $k \geq 2$ and $p > 2$. We first show that $\{\zeta_n\}$ is bounded in $W^{1,p}(S)$. Then assuming $\{\zeta_n\}$ is bounded in $W^{m-1,p}(S)$ for all m where $m - 1 \leq k$ we show $\{\zeta_n\}$ is bounded in $W^{m,p}(S)$. The details follow.

In accordance with Theorem 5.2.3, suppose the sequence $\zeta_n \in W^{k,p}(\Omega)$is bounded independently of n and t with $\|\zeta_n\|_{k,p,\Omega} \in L^1[0,T]$. Then

$$\|\zeta_n\|^p_{0,p,S} = \int_0^T dt\, \|\zeta_n\|^p_{0,p,\Omega} \leq \int_0^T dt\, \|\zeta_n\|^p_{k,p,\Omega} \ , \tag{5.3.3}$$

which is finite and independent of n by Theorem 5.2.3. That is, we have established that $\{\zeta_n\}$ is bounded in $W^{0,p}(S)$. In addition, we have

$$\|\zeta_n\|^p_{1,p,S} = \int_0^T dt\, \left\{\|\zeta_n\|^p_{1,p,\Omega} + \|D_t\zeta_n\|^p_{0,p,\Omega}\right\} \ . \tag{5.3.4}$$

Using equation (5.2.4a) we have

$$\|D_t\zeta_n\|_{1,p,\Omega}^p \leq$$
$$\|v_{n-1}\cdot\nabla\zeta_n\|_{0,p,\Omega}^p + \|F\|_{0,p,\Omega}^p + \|Q \bullet b_n^*\alpha_n\|_{0,p,\Omega}^p \,. \qquad (5.3.5)$$

Using the fact that $W^{1,p}(\Omega)$ is a Banach Algebra for $p > 2$ (Adams, 1975), the first term on the right of inequality (5.3.5) may be estimated by

$$\begin{aligned}\|v_{n-1}\cdot\nabla\zeta_n\|_{0,p,\Omega}^p &\leq \|v_{n-1}\cdot\nabla\zeta_n\|_{1,p,\Omega}^p \\ &\leq \|v_{n-1}\|_{1,p,\Omega}^p\|\nabla\zeta_n\|_{1,p,\Omega}^p \,. \end{aligned}\qquad (5.3.6)$$

Lemma 5.1.2 yields an estimate for v_{n-1}, thus,

$$\|v_{n-1}\cdot\nabla\zeta_n\|_{0,p,\Omega}^p \leq c_1\|\zeta_n\|_{0,p,\Omega}^p\|\zeta_n\|_{2,p,\Omega}^p \,. \qquad (5.3.7)$$

Lemma 5.2.2(b) establishes a bound on $\|Q\bullet b_n^*\alpha_n\|_{0,p,\Omega}^p$ and we have assumed that the forcing, F, satisfies $\|F\|_{k,p,\Omega} \in L_1[0,T]$. Using these bounds, noting that they are independent of n and t, we have $\int_0^T dt\|D_t\zeta_n\|_{1,p,\Omega}^p$ is bounded by the integral over $[0.T]$ of a constant, and thus is finite. From equation (5.3.4) it follows that the sequence $\{\zeta_n\}$ is bounded in $W^{1,p}(S)$, independently of n.

For the induction step, suppose $\{\zeta_n\}$ is bounded independently of n in $W^{j,p}(S)$ for each $j = 1,\ldots,m-1 < k$. Then,

$$\begin{aligned}\|\zeta_n\|_{m,p,S}^p &= \|\zeta_n\|_{m-1,p,S}^p + \sum_{|\alpha|=m}\|D^\alpha\zeta_n\|_{0,p,S}^p \\ &= \|\zeta_n\|_{m-1,p,S}^p + \int_0^T \|\zeta_n\|_{m,p,\Omega}^p + \sum_{l=1}^m\int_0^T \|D_t^l\zeta_n\|_{m-l,p,\Omega}^p \\ &\leq \|\zeta_n\|_{m-1,p,S}^p + \int_0^T \|\zeta_n\|_{k,p,\Omega}^p + c\int_0^T \|\zeta_n\|_{m-1,p,S}^p \,. \end{aligned}\qquad (5.3.8)$$

In each of the terms on the right in inequality (5.3.8), the sequence $\{\zeta_n\}$ is bounded independently of n by the induction hypothesis and Theorem 5.2.3. This concludes the proof.

As a corollary to Theorem 5.3.3, we establish the existence of an EKSM solution. That is, there exists a subsequence of the sequence generated by (4.2.2–3) which converges to a vorticity estimate, ζ^*, which satisfies equation (3.2.6) in the classical sense. The proof is an immediate consequence of the imbedding theorem, Theorem 2.2.1.

Corollary 5.3.4 *Given a sequence $\{\zeta_n\}$ defined by equations (5.2.4–5), $Q \in C^k(\overline{S}) \times C^k(\overline{S})$ and $A \in C^k(\overline{\Omega}) \times C^k(\overline{\Omega})$, and satisfying Theorem 5.3.3, there exists a subsequence, $\{\zeta_{n_i}\}$, converging in $C^j(\overline{S})$ to a limit, $\zeta^* \in C^j(\overline{S})$, where $j = k - m$, provided $mp > n = 3$.*

For a the limit, ζ^* to be a classical solution to equation (5.2.4), that is, $\zeta^* \in C^1(\overline{S})$, we need either $\zeta_n \in W^{2,4}(S)$, $Q \in C^2(\overline{S}) \times C^2(\overline{S})$ and $A \in C^2(\overline{\Omega}) \times C^2(\overline{\Omega})$, or $\zeta_n \in W^{3,3}(S)$, $Q \in C^3(\overline{S}) \times C^3(\overline{S})$ and $A \in C^3(\overline{\Omega}) \times C^3(\overline{\Omega})$.

6. A Comparison of Iterative Schemes

The Generalized Inverse Method (GIM) resulting from the solution of equations (4.1.3–4) (assuming a solution exists) is the result of a formal iterated linearization used as a means for constructing solutions to a nonlinear coupled system (3.2.5–6). Similarly, the Extended Kalman Smoother Method (EKSM) resulting from the solution of (4.2.2–3) was derived using a formal iterated linearization of the nonlinear dynamics (3.1.4). In the following sections we derive two more inverse methods by replacing the formal iterated linearizations leading to GIM and EKSM with formal applications of Newton's method. Newton's method applied to the nonlinear EL equations (3.2.5–6) will be called the Generalized Inverse Method #2 (GIM2). The method derived from application of Newton's method to the model dynamics (3.1.4) will be called the Extended Kalman Smoother Method # 2 (EKSM2).

In comparing these methods we assume that solutions exits and the methods converge. Allowing the iteration index to tend to infinity reveals that GIM, GIM2, and EKSM2 all converge to the nonlinear EL equations (3.2.5–6). EKSM does not converge to the same EL system, suggesting that the iterative linearization leading to the EKSM is in some way too severe. Justification for preferring this "reduced" method (EKSM) to the equivalent methods (GIM, GIM2 and EKSM2) is given in terms of physical arguments and modeling considerations.

The linearizations are easiest to derive by taking a geometric point of view. That is, the differential operators involved in either the model (3.1.4) or the Euler–Lagrange equations (3.2.5–6) must be viewed as smooth maps from an appropriate space into $\mathbb{R}^1$ or $\mathbb{R}^2$. This requires introducing certain definitions to develop a sufficiently abstract vantage point. Since achieving an iterative solution method to circumvent the nonlinearities of these systems is a modest goal, certain technical aspects which may unnecessarily complicate the issues are intentionally omitted. In keeping with this philosophy, the basic definitions are given with the intent of making their relevance to the applications apparent and are therefore not presented in full generality. The general definitions and technical considerations are considered in Olver (1986).

6.1 A second Extended Kalman Smoother Method

Recall that the model includes the dynamical equation (3.1.4), which we repeat here as (6.1.1):

$$\begin{gathered} \zeta_t + v(\zeta)\cdot\nabla\zeta = q(x,t) \\ G\zeta(x,t) = 0, \qquad \text{for} \quad x \in \partial\Omega \\ \zeta(x,0) = \zeta^0(x) + a(x)\ . \end{gathered} \tag{6.1.1}$$

Note that we have assumed that the first-guess forcing, F(x,t) in equation (3.1.4), is zero. This is merely to reduce some of the notational clutter and does not affect the conclusions.

The basic space of three independent variables $(x_1, x_2, t) \in \Omega \times (0,T) = \mathcal{S}$ is a subset of $X := \mathbb{R}^3$. The space of two dependent variables (ζ, q) is in U, a subset of $\mathbb{R}^2$. The basic space of independent and dependent variables is $X \times U$ which is a subset of $\mathbb{R}^5$. In order to achieve the desired geometric vantage point it is necessary to extend the basic space $X \times U$ to a space which represents the various partial derivatives occurring in equation (6.1.1). The set $U_1 \subset \mathbb{R}^6$ represents the space containing coordinates corresponding to the first derivatives of the dependent variables $(\zeta_{x_1}, \zeta_{x_2}, \zeta_t; q_{x_1}, q_{x_2}, q_t)$. A space may now be defined by $U^{(1)} = U \times U_1$ having eight coordinates representing the dependent variables and their first derivatives. An element of $U^{(1)}$ will be denoted by $u^{(1)}$ and has components representing variables given by $(\zeta, q; \zeta_t, \zeta_{x_1}, \zeta_{x_2}, q_t, q_{x_1}, q_{x_2})$.

Given a smooth function $f = f(x,t)$ such that $f : X \mapsto U \subset \mathbb{R}^2$ there is an induced map $f^{(1)} = \mathrm{pr}^{(1)} f(x,t)$ such that $f^{(1)} : X \mapsto U^{(1)}$ called the *first prolongation* of f. Thus, for each (x,t), $\mathrm{pr}^{(1)} f(x,t)$ is a vector whose entries represent the values of f and all its first derivatives at the point (x,t).

The space $X \times U^{(1)}$, whose coordinates represent the independent variables, the dependent variables and the first derivatives of the dependent variables is called the *first order jet space* of the underlying space $X \times U$. We are interested in differential equations defined over some open subset $M \subset X \times U$, for which we denote the first order jet space by $M^{(1)} = M \times U_1$.

The partial differential equation (6.1.1) can be written as

$$\Delta(\vec{x}, u^{(1)}(\vec{x})) = 0 , \qquad (6.1.2)$$

which indicates the dependence of the system on $\vec{x} = (x_1, x_2, t) \in \Omega \times (0,T)$ and $u^{(1)} = (\zeta, q; \zeta_{x_1}, \zeta_{x_2} \zeta_t; q_{x_1}, q_{x_2}, q_t)$. The operator Δ can be viewed as a smooth map from the jet space $M^{(1)} = X \times U^{(1)}$ to $\mathbb{R}^1$,

$$\Delta : M^{(1)} \mapsto \mathbb{R}^1 , \qquad (6.1.3)$$

and is called a *differential function.*

The differential equation (6.1.2) specifies where the map has value zero on $M^{(1)}$, determining what is called a *subvariety* of the space $M^{(1)}$, defined by

$$\Im_\Delta = \{(\vec{x}, u^{(1)}) : \Delta(\vec{x}, u^{(1)}) = 0\} \subset M^{(1)} . \qquad (6.1.4)$$

A smooth function $f(\vec{x}) = f(x,t)$ is a solution of (6.1.2) provided that $\Delta(\vec{x}, \mathrm{pr}^{(1)} f(\vec{x})) = 0$ whenever $\vec{x} = (x,t)$ is in the domain of f. This is equivalent to saying that the graph of the (first) prolongation of f , $\{(\vec{x}, \mathrm{pr}^{(1)} f(\vec{x}))\}$, must lie entirely in the subvariety $\Im_\Delta$. That is,

$$\{(\vec{x}, \mathrm{pr}^{(1)} f(\vec{x}))\} \subset \Im_\Delta = \{\Delta(\vec{x}, \zeta^{(1)}) = 0\} \ . \qquad (6.1.5)$$

We now have in place a reformulation of finding a solution to the partial differential equation (6.1.1) in terms of finding a zero of the map Δ given by (6.1.3). Formally, we may apply Newton's Method to the differential function Δ in an attempt to define a sequence which will converge to a zero of the map. This requires defining the derivative of the map Δ in an applicable fashion.

Let $\mathcal{A}$ denote the space of smooth functions $\Delta(\vec{x}, u^{(1)}(\vec{x}))$ mapping $M^{(1)} \subset X \times U^{(1)}$ into $\mathbb{R}^1$. That is, $\mathcal{A}$ is a space of differential functions. Note that $\mathcal{A}$ is an algebra, meaning that the set is closed under addition and in particular, multiplication.

Let $\Delta(\vec{x}, \zeta^{(1)}(\vec{x})) \in \mathcal{A}$ be a differential function. The *Frechet derivative* of Δ is the differential operator $\mathrm{D}_\Delta : \mathcal{A} \mapsto \mathcal{A}$, defined so that

$$\mathrm{D}_\Delta(G) = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \Delta(\vec{x}, \zeta^{(1)}(\vec{x}) + \epsilon G(\vec{x}, \zeta^{(1)}(\vec{x}))) \qquad (6.1.6)$$

for any differential function $G \in \mathcal{A}$.

For example, to compute the Frechet derivative of the specific Δ given by (6.1.2), replace (ζ, q) and its derivatives by $(\zeta + \epsilon G^1, q + \epsilon G^2)$ and its derivatives. Compute the first derivative with respect to ϵ of the resulting expression and evaluate the derivative at $\epsilon = 0$. Hence, replacing $u = (\zeta, q)$ with $u + \epsilon G = (\zeta + \epsilon G^1, q + \epsilon G^2)$ in the definition of Δ (equations (6.1.1–2) we have

$$\Delta(\vec{x}, u^{(1)} + \epsilon G(\vec{x}, u(1)) = (\zeta + \epsilon G^1)_t + v(\zeta + \epsilon G^1) \cdot \nabla(\zeta + \epsilon G^1) - q - \epsilon G^2 \ , \quad (6.1.7)$$

where $G = (G^1, G^2)$ is any differential function in $\mathcal{A}$. Now computing the derivative with respect to ϵ,

$$\mathrm{D}_\Delta(G) = \frac{d}{d\epsilon}\bigg|_{\epsilon=0} (\zeta + \epsilon G^1)_t + v(\zeta + \epsilon G^1) \cdot \nabla(\zeta + \epsilon G^1) - q - G^2$$
$$= G^1_t + v(G^1) \cdot \nabla\zeta + v(\zeta) \cdot \nabla G^1 - \epsilon G^2 \ . \qquad (6.1.8)$$

We are now in a position to construct Newton's method for finding a zero of the map $\Delta : M^{(1)} \mapsto \mathbb{R}^1$. The method consists of using a linear approximation to Δ at some "prior" estimate, $u^{(1)}_{n-1}$, of the zero and then using the element of $M^{(1)}$ at which the linear map vanishes as the "posterior" estimate, $u^{(1)}_{n-1}$. The process is repeated until convergence ($n \to \infty$) if possible. The linearization of the operator Δ is its Frechet derivative evaluated at the prior estimate, $u^{(1)}_{n-1}$. This leads to the algorithm

$$\Delta(\vec{x}, u^{(1)}_{n-1}) + \mathrm{D}^n_\Delta(u^{(1)}_n - u^{(1)}_{n-1}) = 0 \qquad (6.1.8)$$

where $\mathrm{D}^n_\Delta(G) = G^1_t + v(G^1) \cdot \nabla\zeta_{n-1} + v(\zeta_{n-1}) \cdot \nabla G^1 - G^2$ is the Frechet derivative of Δ evaluated at (ζ_{n-1}, q_{n-1}). Writing the operators explicitly and collecting like terms we obtain the following equation.

$$(\zeta_n)_t + v(\zeta_{n-1}) \cdot \nabla\zeta_n + v(\zeta_n) \cdot \nabla\zeta_{n-1} - v(\zeta_{n-1}) \cdot \nabla\zeta_{n-1} - q_n = 0 \ . \quad (6.1.9)$$

An initial condition must be given for ζ_n and we introduce the initial error, a_n, so that

$$\zeta_n(x, 0) = \zeta^0(x) + a_n \ . \qquad (6.1.10)$$

In analogy with equation (4.2.1) we define the n^{th} cost functional whose minimum will yield the n^{th} best estimate of the n^{th} vorticity in terms of a weighted least squares fit of the (linearized) dynamics (6.1.9) to the data of

(3.1.8). The sequence of cost functionals is defined by

$$\begin{aligned}\mathcal{J}^n(\zeta_n) = &\int_0^T dt \int_\Omega dx \int_0^T dt' \int_\Omega dx' q_n(x,t) W(x,t,x',t') q(x',t') + \\ &+ \int_\Omega dx \int_\Omega dx' a(x) V(x,x') a(x') \\ &+ \epsilon^* w \epsilon \ ,\end{aligned} \tag{6.1.11}$$

where the dependence of $q_n(x,t)$ on $\zeta_n(x,t)$ is, from (6.1.9),

$$q_n(x,t) = (\zeta_n)_t + v(\zeta_{n-1}) \cdot \nabla\zeta_n + v(\zeta_n) \cdot \nabla\zeta_{n-1} - v(\zeta_{n-1}) \cdot \nabla\zeta_{n-1} \ . \tag{6.1.12}$$

The corresponding Euler–Lagrange system of partial differential equations is derived using virtually the same calculations as given in Appendix A for the derivation of equations (3.6.5–6), with appropriate modifications for the equations being used. The result is the system

$$\begin{aligned}(\zeta_n)_t + &v(\zeta_{n-1}) \cdot \nabla\zeta_n + v(\zeta_n) \cdot \nabla\zeta_{n-1} \\ &- v(\zeta_{n-1}) \cdot \nabla\zeta_{n-1} = Q \bullet \mu_n\end{aligned} \tag{6.1.13a}$$

$$\zeta_n(x,0) = \zeta^0(x) + A \circ \mu_n(x,0) \tag{6.1.13b}$$

$$\begin{aligned}-(\mu_n)_t - v(\zeta_{n-1}) \cdot \nabla\mu_n - G[\nabla^\perp\mu_n \cdot \nabla\zeta_{n-1}] \\ = [\mathcal{L}_{(\xi,\tau)}(\delta(x-\xi, t-\tau))]^* w[d - \mathcal{L}(\zeta_n)]\end{aligned} \tag{6.1.14a}$$

$$\mu_n(x,T) = 0 \ . \tag{6.1.14b}$$

Note that solving the system (6.1.13–14) yields an estimate $\hat{\zeta}_n$ which minimizes $\mathcal{J}^n$, equation (6.1.11), since $\mathcal{J}^n$ is quadratic in ζ_n. This is easily verified by computing the second variation of $\mathcal{J}^n$, which results in

$$\begin{aligned}\frac{1}{2}\delta^2\mathcal{J}^n \ = \ & \\ \int_0^T dt \int_\Omega dx \int_0^T dt' \int_\Omega dx' \ & L_n(\xi(x,t) W(x,t,x',t') L_n(\xi(x',t') + \\ &\int_\Omega dx \int_\Omega dx' \ \xi(x,0) V(x,x') \xi(x',0) + \sum_{k,l} \mathcal{L}^k(\xi) w_{kl} \mathcal{L}^l(\xi)\end{aligned} \tag{6.1.15}$$

The method of producing the sequence defined by (6.1.13–14) will be referred to as the Extended Kalman Smoother Method version 2 (EKSM2) to distinguish it from the EKSM defined using (4.2.2–3).

Equations (6.1.13–14) which define EKSM2 are similar to equation (4.1.3–4) which define GIM. The differences being the presence in the adjoint equation of GIM (eq. (4.1.4)) of the term $G[\nabla^{\perp}\mu_{n-1}\cdot\nabla\zeta_{n-1}]$ compared to the term $G[\nabla^{\perp}\mu_{n}\cdot\nabla\zeta_{n-1}]$ in the adjoint equation of EKSM2 (eq. (6.1.14)), and the extra terms in the forward equation of EKSM2 (6.1.13) compared to the forward equation of GIM (4.1.3). The limit of GIM and EKSM2 are both the nonlinear Euler–Lagrange system (3.2.5–6). This is significant because it shows that the iterative linearization leading to EKSM which excludes the terms $v(\zeta_n)\cdot\nabla\zeta_{n-1} - v(\zeta_{n-1})\cdot\nabla\zeta_{n-1}$ from (6.1.9) is resulting in a different type of data smoothing estimate than GIM and EKSM2.

6.2 A second Generalized Inverse Method

Another approach to consider is a linearization using the formal application of Newton's method to the map corresponding to the nonlinear EL equations (3.2.5–6). The basic space of independent and dependent variables is again the set $M \subseteq X \times U \subset \mathbb{R}^5$ representing the coordinates $(x_1, x_2, t; \zeta, \mu)$. The first order jet space, $M^{(1)}$, represents coordinates $(x_1, x_2, t; \zeta, \mu; \zeta_{x_1}, \zeta_{x_2}, \zeta_t; \mu_{x_1}, \mu_{x_2}, \mu_t,)$.

The system of partial differential equations (equations (3.2.5–6)) can now be written as

$$\Delta(\vec{x}, u^{(1)}(\vec{x})) = 0\ , \qquad (6.2.1)$$

involving $\vec{x} = (x_1, x_2, t)$ and $u^{(1)} = (\zeta, \mu; \zeta_{x_1}, \zeta_{x_2}, \zeta_t; \mu_{x_1}, \mu_{x_2}, \mu_t)$. In equation (6.2.1) we consider Δ to be an ordered pair of differential functions, that is, in $\mathcal{A}^2$, of the form $\Delta(\vec{x}, u^{(1)}) = (\Delta_1(\vec{x}, u^{(1)}), \Delta_2(\vec{x}, u^{(1)}))$ where

$$\Delta_1(\vec{x}, u^{(1)}) = \zeta_t + v(\zeta) \cdot \nabla\zeta - Q \bullet \mu \tag{6.2.2}$$

$$\Delta_2(\vec{x}, u^{(1)}) = -\mu_t - v(\zeta) \cdot \nabla\mu - G[\nabla^\perp\mu \cdot \zeta] - \mathcal{L}[\delta]^* w[d - \mathcal{L}(\zeta)] \ . \tag{6.2.3}$$

Applying Newton's method to equation (6.2.1) yields the following iterated system.

$$\Delta(\vec{x}, u^{(1)}_{n-1}) + \mathrm{D}^{n-1}_{\Delta}(u^{(1)}_n - u^{(1)}_{n-1}) = 0 \ . \tag{6.2.4}$$

The Frechet derivative, D_Δ, of the operator Δ is computed as follows. Replace $u^{(1)} = (\zeta^{(1)}, \mu^{(1)})$ with

$$u^{(1)} + \epsilon G^{(1)} = (\zeta^{(1)} + \epsilon G^{(1)}_1, \mu^{(1)} + \epsilon G^{(1)}_2)$$

so that

$$\Delta_1(\vec{x}, u^{(1)} + \epsilon G^{(1)}) = (\zeta + \epsilon G_1)_t + v(\zeta + \epsilon G_1) \cdot \nabla(\zeta + \epsilon G_1) - Q \bullet (\mu - \epsilon G_2) \tag{6.2.5a}$$

$$\Delta_2(\vec{x}, u^{(1)} + \epsilon G^{(1)}) = -(\mu + \epsilon G_2)_t - v(\zeta + \epsilon G_1) \cdot \nabla(\mu + \epsilon G_2) - G[\nabla^\perp(\mu + \epsilon G_2) \cdot \nabla(\zeta + \epsilon G_1)] - \mathcal{L}(\delta)^* w[d - \mathcal{L}(\zeta + \epsilon Q_1)] \ . \tag{6.2.5b}$$

Differentiating the expressions (6.2.5a and b) with respect to ϵ and evaluating at $\epsilon = 0$ we have,

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \Delta_1(\vec{x}, u^{(1)}(\vec{x}) + \epsilon G(\vec{x}, u^{(1)}(\vec{x}))) =$$

$$(G_1)_t + v(G_1)\cdot\nabla\zeta + v(\zeta)\cdot\nabla G_1 - Q \bullet (G_2) \qquad (6.2.6a)$$

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \Delta_2(\vec{x}, u^{(1)}(\vec{x}) + \epsilon G(\vec{x}, u^{(1)}(\vec{x}))) =$$

$$-(G_2)_t - v(G_1)\cdot\nabla(\mu) - v(\zeta)\cdot\nabla Q_2 -$$

$$G[\nabla^{\perp}G_2\cdot\nabla\zeta + \nabla^{\perp}\mu\cdot\nabla Q_1] -$$

$$\mathcal{L}(\delta)^* w[d - \mathcal{L}(Q_1)] \; . \qquad (6.2.6b)$$

We are now in a position to explicitly write (6.2.4) in terms of iterates of ζ and μ. Evaluating (6.2.6) at (ζ_{n-1}, μ_{n-1}) to find $\mathrm{D}_{\Delta}^{n-1}$, applying it to $(\zeta_n^{(1)}, \mu_n^{(1)})$, the algorithm (6.2.4) becomes

$$(\zeta_n)_t + v(\zeta_{n-1})\cdot\zeta_n + v(\zeta_n)\cdot\zeta_{n-1} -$$

$$v(\zeta_{n-1})\cdot\zeta_{n-1} - Q \bullet \mu_n = 0 \qquad (6.2.7a)$$

$$-(\mu_n)_t - v(\zeta_{n-1})\cdot\mu_n - v(\zeta_n)\cdot\mu_{n-1} + v(\zeta_{n-1})\cdot\mu_{n-1} -$$

$$G[\nabla^{\perp}\mu_n\cdot\nabla\zeta_{n-1} + \nabla^{\perp}\mu_{n-1}\cdot\nabla\zeta_n - \nabla^{\perp}\mu_{n-1}\cdot\nabla\zeta_{n-1}] -$$

$$\mathcal{L}[\delta]^* w[d - \mathcal{L}(\zeta_n)] = 0 \qquad (6.2.7b)$$

The initial condition for the vorticity iterate, $\zeta_n(x,0)$, and the final condition for the adjoint variable, $\mu_n(x,T)$ are given by the EL system (3.2.6b,7b).

$$\zeta_n(x,0) = \zeta^0 + A \circ \mu_n(x,0) \qquad (6.2.8)$$

$$\mu_n(x,T) = 0 \qquad (6.2.9)$$

For convenience of reference we collect each of the methods (GIM, GIM2, EKSM, and EKSM2) on the following pages.

GIM: Generalized Inverse Method (eq.(4.1.3–4),

$$(\zeta_n)_t + v(\zeta_{n-1}) \cdot \nabla\zeta_n = F + Q \bullet \mu_n \tag{6.2.10a}$$

$$\zeta_n(x,0) = \zeta^0(x) + A \circ \mu_n(x,0) \tag{6.2.10b}$$

$$-(\mu_n)_t - v(\zeta_{n-1}) \cdot \nabla\mu_n - G[v(\Delta\mu_{n-1}) \cdot \nabla\zeta_{n-1}] = \tag{6.2.11a}$$

$$[\mathcal{L}_{(\xi,\tau)}(\delta(x-\xi)\delta(t-\tau))]^* w[d - \mathcal{L}(\zeta_n)]$$

$$\mu_n(x,T) = 0\ . \tag{6.2.11b}$$

GIM2: Generalized Inverse Method version 2 (eq.(6.2.6–9),

$$(\zeta_n)_t + v(\zeta_{n-1}) \cdot \zeta_n + v(\zeta_n) \cdot \zeta_{n-1} -$$

$$v(\zeta_{n-1}) \cdot \zeta_{n-1} = Q \bullet \mu_n \tag{6.2.12a}$$

$$\zeta_n(x,0) = \zeta^0 + A \circ \mu_n(x,0) \tag{6.2.12b}$$

$$-(\mu_n)_t - v(\zeta_{n-1}) \cdot \nabla\mu_n - v(\zeta_n) \cdot \nabla\mu_{n-1} + v(\zeta_{n-1}) \cdot \nabla\mu_{n-1} -$$

$$G[\nabla^\perp\mu_n \cdot \nabla\zeta_{n-1} + \nabla^\perp\mu_{n-1} \cdot \nabla\zeta_n - \nabla^\perp\mu_{n-1} \cdot \nabla\zeta_{n-1}] -$$

$$\mathcal{L}[\delta]^* w[d - \mathcal{L}(\zeta_n)] = 0 \tag{6.2.13a}$$

$$\mu_n(x,T) = 0 \tag{6.2.13b}$$

EKSM: Extended Kalman Smoother Method (eq.(4.2.2–3),

$$(\zeta_n)_t + v(\zeta_{n-1}) \cdot \nabla\zeta_n = F + Q \bullet \mu_n \tag{6.2.14a}$$

$$\zeta_n(x,0) = \zeta^0(x) + A \circ \mu_n(x,0) \tag{6.2.14b}$$

$$-(\mu_n)_t - v(\zeta_{n-1}) \cdot \nabla\mu_n = \tag{6.2.15a}$$

$$[\mathcal{L}_{(\xi,\tau)}(\delta(x-\xi)\delta(t-\tau))]^* w[d - \mathcal{L}(\zeta_n)]$$

$$\mu_n(x,T) = 0\ . \tag{6.2.15b}$$

EKSM2: Extended Kalman Smoother Method version 2 (eq.(6.1.13–14),

$$(\zeta_n)_t + v(\zeta_{n-1}) \cdot \nabla\zeta_n + v(\zeta_n) \cdot \nabla\zeta_{n-1} - v(\zeta_{n-1}) \cdot \nabla\zeta_{n-1} = Q \bullet \mu_n \qquad (6.1.16a)$$

$$\zeta_n(x,0) = \zeta^0(x) + A \circ \mu_n(x,0) \qquad (6.1.16b)$$

$$-(\mu_n)_t - v(\zeta_{n-1}) \cdot \nabla\mu_n - G[\nabla^\perp\mu_n \cdot \nabla\zeta_{n-1}] = [\mathcal{L}_{(\xi,\tau)}(\delta(x-\xi, t-\tau))]^* w[d - \mathcal{L}(\zeta_n)] \qquad (6.1.16a)$$

$$\mu_n(x,T) = 0 \ . \qquad (6.1.16b)$$

The derivations of each of these methods are summarized as follows. In an effort to smooth the given data d, defined in equation (3.1.8), using the nonlinear model (3.1.4) there are two basic approaches considered here. One approach is to define a cost functional using a weighted mean squared model error, initial error and data error. Deriving the Euler–Lagrange equations whose solution corresponds to a necessary condition for a minimum leads to a nonlinear boundary–value (space and time) problem (3.2.5–6). One method of iterating this system leads to the Generalized Inverse Method (GIM). As an alternative iterative method, a formal application of Newton's method may be applied to the nonlinear system resulting in the Generalized Inverse Method version 2 (GIM2).

Another approach used to smooth the data is to first linearize the model, and then define a sequence of minimization problems of which each iterate obtains the best least–squares fit of a linearized model to the data. One method of iterating was given in (4.2.2–3) is the Extended Kalman Smoother Method (EKSM). An alternative iterative method is to formally apply Newton's method to obtain an iterated model (eq.(6.1.9–10)) resulting in the

Extended Kalman Smoother version 2 (EKSM2).

The primary objective of data assimilation is to obtain an estimate $\hat{\zeta}$ of the state of the vorticity at each space–time point (x, t) in the fixed domain $\overline{S} = \overline{\Omega} \times [0, T]$. Any of the above methods, in principle, will provide such an estimate. Furthermore, if the sequences generated by each of the methods converge, then GIM, GIM2, and EKSM2 provide the same estimate since in the limit each of these methods converges to the EL system (3.2.5–6). The estimate provided by EKSM will, in principle, differ from the estimate provided by the other methods. Yet, by the argument which follows, it is EKSM which is the most attractive scheme from a modeling point of view.

Any presence of terms of the form $v(\zeta_n) \cdot \nabla\zeta_{n-1}$ in the forward integration allows for the formation of a barotropic instability with exponential growth in amplitude with time (Pedlosky, 1987). This mechanism extracts energy from the mean flow of the $(n-1)^{\text{st}}$ iterate and feeds it into the n^{th} iterate. Similarly, the presence of terms such as $\nabla^{\perp}\mu_n \cdot \nabla\zeta_{n-1}$ provide a mechanism for the growth of "energy" in the adjoint variable, μ_n, leading to unstable forcing in the forward equation governing ζ_n. These terms are present in GIM2 and EKSM2. Even GIM contains the term $\nabla^{\perp}\mu_{n-1} \cdot \nabla\zeta_{n-1}$, which provides a potential feedback mechanism for the forcing on successive iterates. It is the presence of these terms and the mechanisms for instability which are associated to them that indicates that showing that the sequence of solutions generated by GIM2, EKSM2, and GIM are bounded is not likely to be accomplished.

7. Summary and Discussion

Chapter 1 is a general introduction to the scope of this thesis. Chapter 2 establishes the notation and collects pertinent definitions and theorems which are used throughout.

Chapter 3 is a description of one approach for constructing a generalized inverse of the two–dimensional, incompressible Euler equations when observed data are available. The resulting estimate of vorticity smooths the (sparse) data over a fixed space–time domain. The method is a control theory approach in which control functions are introduced into the forcing and initial condition of the vorticity equation. The problem is to then minimize a cost functional consisting of a sum of weighted L^2–norms of the controls plus a weighted squared misfit to the data. A vorticity estimate must satisfy the corresponding Euler–Lagrange equations if it is to minimize the cost functional. Solving the Euler–Lagrange system is the way in which the estimates are produced in the context of this paper. The nonlinear nature of the vorticity dynamics presents some difficulties. One is that the cost functional is not convex in its dependence on the vorticity and so an extremum of the cost is not necessarily a local minimum, or even a local minimum. Another difficulty is that the Euler–Lagrange equations are nonlinear, in addition to being a coupled system and having initial, final, and spatial boundary conditions. An iteration method which provides a means to solve this system (GIM) is described in Chapter 4.

The fact that the nonlinear Euler–Lagrange equations must be solved using an iterative scheme motivated a reformulation of the control problem: iterate the vorticity equation (to linearize) and then form a sequence of quadratic cost functionals. The sequence of cost functionals has a corresponding sequence of linear Euler–Lagrange systems (EKSM; section 4.2).

Section 4.3 contains a means for constructing solutions to the systems of partial differential equations defined by GIM and EKSM. The construction is accomplished by writing the vorticity estimates as a sum of a first–guess solution plus a linear combination of representer functions. The representer functions are dependent on the structure of the measurement functionals and the dynamics. The representers completely characterize the influence of the observing system (i.e. measurement functionals) in the following sense. The first–guess, ζ_{F_n}, and the representers, r_n, span a finite dimensional space, span$\{\zeta_{F_n}, r_n\}$. Any field orthogonal to span$\{\zeta_{F_n}, r_n\}$ (in the sense of the inner product defined in equation (C1)) is unobservable, meaning that its measured values are zero (Bennett and Thorburn, 1992, Bennett, 1990). The coefficients in the linear combination are determined by measurements of the representer functions, and by the discrepancy between the observed data and the measured first–guess.

In Theorem 5.3.3 of Chapter 5, the sequence of vorticity estimates obtained from EKSM, $\{\zeta_m\}$, was shown to be bounded in the Sobolev space $W^{k,p}(S)$. This holds for $k \geq 2$, $p > 2$, and under mild restrictions on the first iterate, $\zeta_0(x,t)$, the initial condition, $\zeta^0(x)$, and the covariance kernels $Q(x,t,x',t')$ and $A(x,x')$. The strategy used to obtain the bound was to first show that the sequence is bounded in $W^{k,p}(\Omega)$ with $\|\zeta_n\|_{k,p,\Omega} \in L^1[0T]$. Then the bound in $W^{k,p}(S)$ was achieved using an induction argument and relying on the specific properties of the partial differential equation governing the vorticity estimate (4.2.2–3). The main result of this paper is the proof of the existence of an estimate of vorticity resulting from EKSM (Corollary 5.3.4). The proof of existence of a solution establishes EKSM as a viable method for applications. The shortcomings of applying a method for which existence of a solution is uncertain is obvious.

In EKSM, the first–guess vorticity, ζ_{Fn}, is not influenced by the control parameters since the first–guess adjoint, μ_{F_n}, is identically zero (see equations (4.3.3–4) and (5.2.1–3)). In contrast, the first–guess vorticity of GIM *does* depend on the control parameters since $\mu_{F_n} \neq 0$. This difference in the first–guess solutions obtained from GIM and EKSM is one of the significant features which allowed the proof of existence of an EKSM solution and prevented us from obtaining a bound on the sequence generated by GIM. In Chapter 6 we have argued that certain instability mechanisms which are formally present in GIM, may prevent the sequence of vorticity estimates from being bounded as iteration progresses. Bennett and Thorburn (1992) have shown GIM diverges for a numerically simulated quasi–geostrophic model.

The relationship between EKSM and GIM was explored in Chapter 6 in terms of formal applications of Newton's method. Again there are two approaches. One is to apply Newton's method to the (nonlinear) Euler-Lagrange equations. This resulted in the method referred to as GIM2. The other approach is to first use Newton's method to iterate the vorticity equation resulting in a sequence of cost functionals. Solution of the corresponding sequence of (linear) Euler–Lagrange equations results in the method referred to as EKSM2. These two approaches (GIM2 and EKSM2) are equivalent in the sense that in the limit, as the iteration index tends to infinity, both of the linear iterated Euler–Lagrange systems converge to the nonlinear Euler–Lagrange system. (This is also true of GIM). The linear iterated Euler–Lagrange system in EKSM does not converge to the nonlinear system since the iterative method leaves out some terms which are present in the formal application of Newton's method. However, the forward equation of EKSM does converge to the forward equation of the nonlinear Euler–Lagrange system. That is, EKSM provides a vorticity estimate consistent with the nonlinear dynamical problem, but the nature of the applied controls is somewhat different than those provided by GIM, GIM2, or EKSM2. Furthermore, the presence of instability mechanisms in each of GIM, GIM2, and EKSM2 leaves EKSM as being the most robust, supported by our proof of existence of a solution using EKSM.

The theory for linear finite and infinite dimensional control problems is well developed. The theory for nonlinear finite dimensional control problems has been considered from a stochastic processes point of view, utilizing statistical linearizations (Gelb, 1974). We have provided an existence proof for a nonlinear infinite dimensional (deterministic) control problem. The techniques were motivated by existence proofs for models of two–dimensional, incompressible fluids (Judovič, 1966a, Bennett and Kloeden, 1980). The opportunity to extend the existence proof of EKSM to more complicated fluid models depends on the availability of existence proofs for the models themselves. The proof relies on the specific nature of the system of partial differential equations to establish the required differential inequalities. It would not be difficult to extend the results to a quasi–geostrophic channel model, which is useful for local–area ocean and atmosphere modeling.

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APPENDIX

Appendix A

A1. Derivation of the Euler–Lagrange system

The dynamics are considered to be the vorticity equation for two-dimensional, incompressible flow

$$\begin{aligned} \zeta_t + v(\zeta)\cdot\nabla\zeta &= F(x,t) + q(x,t) \\ G\zeta(x,t) &= 0, \qquad \text{for } x \in \partial\Omega \\ \zeta(x,0) &= \zeta^0(x) + a(x) \ , \end{aligned} \tag{A1.1.1}$$

where G is the Greens function operator associated with the Dirichlet problem

$$\begin{aligned} \Delta\psi &= \zeta \quad \text{in } \Omega \\ \psi &= 0 \quad \text{on } \partial\Omega \ , \end{aligned} \tag{A1.1.2}$$

at each time t. That is,

$$\psi = G\zeta \ . \tag{A1.1.3}$$

The velocity field, $v(\zeta)$, in (A1.1.1) is the divergence free vector field given by $\nabla^{\perp}(G(\zeta)) = (-(G\zeta)_y, (G\zeta)_x)$.

The measurement functionals are linear functionals acting on elements of $W^{k,p}(\mathcal{S})$ (the space of vorticity distributions) and have the form

$$\mathcal{L}^k(\zeta) = \int_0^T dt \int_\Omega dx \mathcal{K}^k(x,t,x_k,t_k) G\zeta(x,t) \ . \tag{A1.2.1}$$

We consider the measurement operator to be a smoothing operator, by considering the kernel $\mathcal{K}^k$ to be a smooth function localized about the point (x_k, t_k).

The cost functional to be minimized over all $\zeta \in \{\xi \in W^{k,p}(\Omega) : G\xi = 0 \text{ on } \partial\Omega\}$ is given by

$$\mathcal{J}(\zeta) = \int_0^T dt' \int_\Omega dx' \int_0^T dt \int_\Omega dx\, q(x,t) W(x,t,x',t') q(x',t') + \int_\Omega dx' \int_\Omega dx\, a(x) V(x,x') a(x') + \sum_{k,l} [d^k - \mathcal{L}^k(\zeta)] w_{kl} [d^l - \mathcal{L}^l(\zeta)] \; . \qquad (A1.3.1)$$

The functional variations ξ must be of the same class as ζ, and therefore must satisfy $G\xi(x,t) = 0$ for $x \in \partial\Omega$. We have that

$$\mathcal{J}(\zeta + \epsilon\xi) = \qquad (A1.3.2)$$

$$\int_0^T dt' \int_\Omega dx' \int_0^T dt \int_\Omega dx \Big\{ \big[\zeta_t + v(\zeta + \epsilon\xi) \cdot \nabla(\zeta + \epsilon\xi)) - F\big] W(x',t',x,t) \times \big[\zeta_t + v(\zeta + \epsilon\xi) \cdot \nabla(\zeta + \epsilon\xi)) - F\big] \Big\} +$$

$$\int_\Omega dx' \int_\Omega dx \, [\zeta(x,0) + \epsilon\xi(x,0) - \zeta^0(x)] \, V(x,x') \, [\zeta(x',0) + \epsilon\xi(x',0) - \zeta^0(x')] +$$

$$\sum_{k,l} [d^k - \mathcal{L}^k(\zeta + \epsilon\xi)] w_{kl} [d^l - \mathcal{L}^l(\zeta + \epsilon\xi)] \; .$$

Taking the derivative of $\mathcal{J}(\zeta + \epsilon\xi)$ with respect to ϵ, and using the assumption that W and V are symmetric with respect to the primed and unprimed arguments,

$$\frac{1}{2}\frac{d}{d\epsilon}\mathcal{J} = \qquad (A1.3.3)$$

$$\int_0^T dt \int_\Omega dx \int_0^T dt' \int_\Omega dx' \Big\{ [\xi_t + v(\xi) \cdot \nabla(\zeta + \epsilon\xi) + (v(\zeta) + \epsilon v(\xi)) \cdot \nabla\xi] \times W(x,t,x',t') [\zeta_t + \epsilon\xi_t + v(\zeta + \epsilon\xi) \cdot \nabla(\zeta + \epsilon\xi) - F] \Big\} +$$

$$\int_\Omega dx \int_\Omega dx' \Big\{ \xi(x,0) V(x,x') [\zeta(x',0) + \epsilon\xi(x',0) - \zeta^0(x')] \Big\} +$$

$$\sum_{kl}\left\{\mathcal{L}^k(\xi)w_{kl}[\mathcal{L}^l(\zeta+\epsilon\xi)-d^l]\right\}.$$

In the limit as $\epsilon\rightarrow 0$, we have the first variation of the cost functional,

$$\frac{1}{2}\delta\mathcal{J}= \tag{A1.3.4}$$

$$\int_0^T dt\int_\Omega dx\int_0^T dt'\int_\Omega dx'\left\{[\xi_t+v(\xi)\cdot\nabla\zeta+v(\zeta)\cdot\nabla\xi]W(x,t,x',t')\times\right.$$

$$\left.[\zeta_t+v(\zeta)\cdot\nabla\zeta)-F]\right\}+$$

$$\int_\Omega dx\int_\Omega dx'\left\{\xi(x,0)V(x,x')[\zeta(x',0)-\zeta^0(x')]\right\}+$$

$$\sum_{kl}\left\{\mathcal{L}^k(\xi)w_{kl}[\mathcal{L}^l(\zeta)-d^l]\right\}.$$

The adjoint variable, $\mu(x,t)$ is defined to be the weighted forcing error, that is,

$$\begin{aligned}\mu(x,t)&=\int_0^T dt'\int_\Omega dx' W(x,t,x',t')q(x',t')\\&=\int_0^T dt'\int_\Omega dx' W(x,t,x',t')[\zeta_t+v(\zeta)\cdot\nabla\zeta)-F]\end{aligned} \tag{A1.3.5}$$

The first variation of the cost functional can then be written

$$\frac{1}{2}\delta\mathcal{J}= \tag{A1.3.6}$$

$$\int_0^T dt\int_\Omega dx[\xi_t+v(\xi)\cdot\nabla\zeta+v(\zeta)\cdot\nabla\xi]\mu(x,t)+$$

$$\int_\Omega dx\int_\Omega dx'\left\{\xi(x,0)V(x,x')[\zeta(x',0)-\zeta^0(x')]\right\}+$$

$$\sum_{kl}\left\{\mathcal{L}^k(\xi)w_{kl}[\mathcal{L}^l(\zeta)-d^l]\right\}.$$

Integration by parts yields

$$\frac{1}{2}\delta\mathcal{J} = \tag{A1.3.6}$$

$$\int_0^T dt \int_\Omega dx \Big\{ \big[-\mu_t - v(\zeta)\cdot\nabla\mu - G(\nabla^\perp\mu\cdot\nabla\zeta) +$$

$$\sum_{kl}\{\mathcal{L}^k(\delta(x-x',t-t'))w_{kl}[\mathcal{L}^l(\zeta)-d^l]\}\big]\xi\Big\} +$$

$$\int_\Omega dx \Big\{ \int_\Omega dx' V(x,x')[\zeta(x',0)-\zeta^0(x')-\mu(x',0)]\Big\}\xi(x,0) +$$

$$\int_\Omega dx[\mu(x,T)\xi(x,T)] \ ,$$

where the measurement term has been obtained by observing the following relation.

$$\mathcal{L}^k(\xi(x,t)) \tag{A1.3.7}$$

$$= \int_0^T dt \int_\Omega dx \mathcal{K}^k(x,t,x_k,t_k)G(\xi(x,t))$$

$$= \int_0^T dt \int_\Omega dx \Big\{ \mathcal{K}^k(x,t,x_k,t_k)G \int_0^T dt' \int_\Omega dx' \Big\{ \xi(x',t')\delta(x-x',t-t')\Big\}$$

$$= \int_0^T dt \int_\Omega dx \int_0^T dt' \int_\Omega dx' \xi(x',t')\mathcal{K}^k(x,t,x_k,t_k)G[\delta(x-x',t-t')]$$

$$= \int_0^T dt \int_\Omega dx \int_0^T dt' \int_\Omega dx' \xi(x,t)\mathcal{K}^k(x',t',x_k,t_k)G[\delta(x-x',t-t')]$$

$$= \int_0^T dt \int_\Omega dx \xi(x,t)\mathcal{L}^k[\delta(x-x',t-t')] \ .$$

We have used the following property of the integral operator G,

$$\int_0^T dt \int_\Omega dx G(\xi) f(x,t) = \int_0^T dt \int_\Omega dx \int_\Omega dx' g(x,x')\xi(x',t) f(x,t) \tag{A1.3.8}$$

$$= \int_0^T dt \int_\Omega dx \int_\Omega dx' g(x', x)\xi(x, t) f(x', t)$$

$$= \int_0^T dt \int_\Omega dx \xi G(f) \ .$$

For variations ξ, in the class $\{\xi \in W^{k,p}(S) \ : \ G\xi = 0 \text{ on } \partial\Omega\}$ (with $k \geq 2$ and $p \geq 4$ or $k \geq 3$ and $p \geq 2$), a necessary condition for $\delta\mathcal{J} = 0$ is that μ satisfy the following equation.

$$-\mu_t - v(\zeta) \cdot \nabla\mu - G[\nabla^\perp \mu] - \sum_{kl} \left\{ \mathcal{L}^k(\delta(x - x', t - t')) w_{kl} [d^l - \mathcal{L}^l(\zeta)] \right\} = 0 \ . \qquad (A1.3.9)$$

Assuming that we have such a μ, the first variation of the cost functional is reduced to

$$\int_\Omega dx \left\{ \int_\Omega dx' V(x, x')[\zeta(x', 0) - \zeta^0(x') - \mu(x, 0)] \right\} \xi(x, 0) + \int_\Omega dx [\mu(x, T)\xi(x, T)] \ , \qquad (A1.3.10)$$

from which the following initial and final conditions are deduced to be necessary.

$$\mu(x, 0) = \int_\Omega dx' V(x, x')[\zeta(x', 0) - \zeta^0(x')] \qquad (A1.3.11)$$

$$\mu(x, T) = 0 \qquad (A1.3.12)$$

The initial condition for μ in equation (A1.3.11) may be changed into an initial condition for ζ by multiplying (A1.3.11) by $A(x, x')$ and using the functional inverse property (3.2.3). This yields the condition on $\zeta(x, 0)$,

$$\zeta(x, 0) = \zeta^0(x) + A \circ \mu(x, 0) \ , \qquad (A1.3.13)$$

where $A \circ \mu$ is as given by (3.2.9).

We now have a system of equations given by the dynamics (A1.1.1), with the initial condition (A1.3.13), and the adjoint equation to the dynamics (A1.3.9), with the final condition (A1.3.12). This is the system given in (3.2.6–7).

Appendix B

B1. Uniqueness of solutions for each iterate

We will show that a solution to the system given by equations (4.1.9–10) or by equations (4.2.2–3) must be unique. For convenience of notation we will assume that the iteration index, n, is fixed and disregard it in the notation. Instead we will denote $v(\zeta_{n-1})$ by U, J_{n-1} by $\bar{J}$ and L_{n-1} by L. That is,

$$\begin{aligned} L(\eta) &= \eta_t + U \cdot \nabla(\eta) \\ &= \eta_t + v(\zeta_{n-1}) \cdot \nabla(\eta) \ . \end{aligned} \tag{B1}$$

With this notation, (4.1.9–10) is written as

$$L\zeta = F + Q \bullet \mu \tag{B2.a}$$

$$\zeta(x,0) = \zeta^0(x) + A \circ \mu(x,0) \tag{B2.b}$$

$$-L\mu = \bar{J} + [\mathcal{L}_{(\xi,\tau)}(\,\delta(x-\xi)\delta(t-\tau))]^* w[d - \mathcal{L}(\zeta)] \tag{B3.a}$$

$$\mu(x,T) = 0\ . \tag{B3.b}$$

Suppose that (ζ^1, μ^1) and (ζ^2, μ^2) are each solutions to (B2–B3). Then their difference $(\zeta, \mu) = (\zeta^1 - \zeta^2, \mu^1 - \mu^2)$ must satisfy

$$L\zeta = Q \bullet \mu \tag{B4.a}$$

$$\zeta(0) = A \circ \mu(x,0) \tag{B4.b}$$

$$-L\mu = [\mathcal{L}_{(\xi,\tau)}(\,\delta(x-\xi)\delta(t-\tau))]^* w[-\mathcal{L}(\zeta)] \tag{B5.a}$$

$$\mu(x,T) = 0 \tag{B5.b}$$

Notice that if we had started instead with equations (4.2.2–3) this equation still holds since the term $\overline{J}$ has dropped out. Therefore what follows applies to either GIM or EKSM.

Multiplying (B5.a) by ζ and integrating by parts over $\Omega \times [0,T]$ we obtain

$$\int_0^T dt \int_\Omega dx (L\zeta)\mu + \int_\Omega dx \zeta(x,0)\mu(x,0) + \mathcal{L}(\zeta)^* w \mathcal{L}(\zeta) = 0 \; . \tag{B6}$$

Substituting into B6, using B4.a we have

$$\int_0^T dt \int_\Omega dx (Q\bullet)\mu + \int_\Omega dx (A \circ \mu(x,0))\mu(x,0) + \mathcal{L}(\zeta)^* w \mathcal{L}(\zeta) = 0 \; . \tag{B7}$$

That is,

$$\begin{aligned} &\int_0^T dt \int_\Omega dx \int_0^T dt' \int_\Omega dx' \mu(x,t) Q(x,t,x',t') \mu(x',t') \\ &\qquad + \int_\Omega dx \int_\Omega dx' \mu(x,0) A(x,x') \mu(x,0) \\ &\qquad + \mathcal{L}(\zeta)^* w \mathcal{L}(\zeta) = 0 \; . \end{aligned} \tag{B8}$$

Equation (B8) shows that a quadratic functional is equal to zero, which is possible only if each of the positive terms in the sum is zero. Consequently,

$$\mu(x,t) \equiv 0 \quad \text{and} \quad \mathcal{L}(\zeta) \equiv 0 \; . \tag{B9}$$

Then (B4) reduces to

$$\begin{aligned} L\zeta &= 0 \\ \zeta(x,0) &= 0 \; , \end{aligned} \tag{B10}$$

which implies

$$\zeta(x,t) \equiv 0 \; . \tag{B11}$$

We conclude that $\zeta^1 = \zeta^2$ and $\mu^1 = \mu^2$, proving uniqueness of solutions for the linear system (B2–3). As a consequence, we have shown uniqueness for either GIM (4.1.9–10) or EKSM (4.2.2–3).

Appendix C

Some properties of representers

Let $a(x,t)$ and $b(x,t)$ be functions in $W^{k,p}(S)$ with $div\,(Ga) = div\,(Gb) = 0$ for all $t \in [0,T]$. Define the mapping $\langle\cdot,\cdot\rangle_n$ from $W^{k,p}(S) \times W^{k,p}(S)$ into $\mathbb{R}^1$ by

$$\langle a,b\rangle_n = \int_0^T dt' \int_\Omega dx' \int_0^T dt \int_\Omega dx\, L_n a(x,t) W(x,t,x't') L_n b(x',t') + \int_\Omega dx' \int_\Omega dx\, a(x,0) V(x,x') b(x,0) \ . \tag{C1}$$

Since W and V are symmetric, positive definite functions (see equation (3.2.2), the relation $\langle\cdot,\cdot\rangle_n$ is an inner product on $W^{k,p}(S)$ (not necessarily equivalent to the usual inner product). Using the representer equations (4.3.1–2) and integration by parts we have for any $\zeta \in W^{k,p}(S)$ (Bennett and Thorburn, 1992, Bennett, 1990),

$$\langle r_n^j, \zeta\rangle_n = \mathcal{L}^j(\zeta) \ . \tag{C2}$$

Define the cost functional, $C^n(\zeta)$, by,

$$C^n(\zeta) = \langle \zeta - \zeta_{F_n}, \zeta - \zeta_{F_n}\rangle_n + [d - \langle r_n, \zeta\rangle_n]^* w [d - \langle r_n, \zeta\rangle_n] \ , \tag{C3}$$

where ζ_{F_n} satisfies equation (4.3.3).

An easy check using equation (4.3.3) to substitute for ζ_{F_n}, and (C2) to substitute for $\langle r_n, \zeta\rangle_n$ shows that the Euler–Lagrange system corresponding to the cost functional C^n is the system (4.2.2–3). Hence, the vorticity estimates which are extremals of C^n are also extremals of J^n (and vice versa). This allows a geometric interpretation of EKSM.

The representer functions, r_n^j, together with the first–guess, ζ_{F_n}, span a finite dimensional subspace of $W^{k,p}(S)$ of at most dimension M. Thus, we can write $\zeta \in W^{k,p}(S)$ as the first–guess plus a linear combination of the representers, plus a function $g_n(x,t)$ which is orthogonal to all of the r_n^j's in the sense that $\langle r_n^j, g_n \rangle_n = 0$.

$$\zeta = \zeta_{F_n} + b_n^* r_n + g_n \; . \tag{C4}$$

From equation (C2) we see that g_n being orthogonal to r_n means that g_n is unobservable—all of its measured values are zero.

Substituting the expansion (C4) into the cost functional (C3) it is possible to obtain the following form (Bennett, 1990,Bennett and Thorburn, 1992).

$$C^n(\zeta) = [b_n - \hat{b}_n*]^* S_n [b_n - \hat{b}_n] + \langle g_n, g_n \rangle_n + h_n^* P_n^{-1} h_n \; , \tag{C5}$$

where $\hat{b}_n = P_n^{-1}$ is the ESKM estimate for b_n (4.3.10), $S_n = R_n + R_n w R_n$, R_n being the representer matrix given by (4.3.9), $P_n = R_n + w^{-1}$ from equation (4.3.8), and $h_n = d - \mathcal{L}(\zeta_{F_n})$ as in equation (4.3.7). The point of obtaining the cost functional (C3) in the form of equation (C5) is that it provides a geometric interpretation of the minimization problem. By choosing $b_n = \hat{b}_n$, and $g_n(x,t) = 0$ we obtain the minimum cost, $\min C^n = h^* P^{-1} h_n = [d - \mathcal{L}(\zeta_{F_n})][R_n + w^{-1}]^{-1}[d - \mathcal{L}(\zeta_{F_n})]$. The choice $b_n = \hat{b}_n$ means that the optimal (in the sense of minimum cost) representer coefficients are given by solving the linear system in equation (4.3.6) corresponding to the EKSM solution. Choosing $g_n(x,t) = 0$ implies that no unobservable field is included in the inverse.