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RESIDUAL MODELS FOR NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS

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Abstract. Residual terms that appear in nonlinear PDEs that are constructed to generate filtered representations of the variables of the fully resolved system are examined by way of a consistency condition. It is shown that certain commonly used empirical gradient models for the residuals fail the test of consistency and therefore cannot be validated as approximations in any reliable sense. An alternate method is presented for computing the residuals. These residual models are independent of free or artificial parameters and there direct link with the functional form of the system of PDEs which describe the fully resolved system are established.

1. Introduction

Nonlinear systems of PDEs can generate solutions that exhibit multiscale fluctuations. When numerical methods are used as the solution method the discretization of the solution domain will result in a loss of resolution of the finer scale fluctuations. The macroscopic equations that are constructed to generate some kind of filtered representation of the fully resolved variables contain residual terms that attempt to model mechanisms that are manifestations of some microscopic process. Here we shall examine a number of residual models for nonlinear PDE systems in common use today, which we shall refer to as empirical gradient models. It will be shown on the basis of a consistency condition alone that these models cannot be regarded as residual approximations in any reasonable sense.

Some of the results presented here appear in [5] but have been recast in a setting of contact manifolds where the base manifold is space/time/scale. This is done because in such a setting analysis of nonlinear PDEs appears more natural and a new level of insight into the derivations is gained from a geometric perspective. We start with a few preliminary details of contact manifolds that will be adequate for our purposes. For a more rigorous development of integral manifolds of distributions on contact manifolds see for instance [9].

Let $x = (x^1, \dots, x^n)$ represent the cartesian coordinates of the n-dimensional space domain $\mathbb{R}^n$ $(n = 1, 2, 3)$, $t \in (0, t_0)$ the time, where $t_0 > 0$, and $\eta \in (0, \eta_0)$ the scale parameter, where $0 < \eta_0 \ll 1$. Set $M \subset \mathbb{R}^m$, $m = n + 2$, such that

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$M = \mathbb{R}^n \times (0,t_0) \times (0,\eta_0)$ with coordinates on M represented by $(x,t,\eta) = (x^1,\dots,x^n,t,\eta)$, where x^k $(k=1,\dots,n)$ are the spatial coordinates, $x^{n+1}=t$ is the time coordinate and $x^{n+2}=\eta$ is the scale coordinate. It is important to keep in mind that we use the symbol x to refer only to the spatial component of $(x^i) = (x,t,\eta) = (x^1,\dots,x^n,t,\eta)$.

Let $K \subseteq \mathbb{R}^{m+N+Nm+Nm^2}$ denote the second order contact manifold whose coordinates are given by $(x^i, u^\alpha, u^\alpha_i, u^\alpha_{ij})$, $1 \le \alpha \le N$, $1 \le i,j \le m = n+2$. We associate u^α as placeholders for the solutions of PDEs and u^α_i and u^α_{ij} as the placeholders for the first and second partial derivatives of u^α. As components of the coordinates of K they are independent variables.

The natural basis for the tangent space $T(M)$ of the base manifold M is $\{\partial_i\}_{1\le i\le m}$ and the natural basis of the tangent space $T(K)$ of K is $\{\partial_i, \dot\partial_\alpha, \dot\partial^i_\alpha, \dot\partial^{ij}_\alpha\}_{1\le i,j\le m; 1\le\alpha\le N}$, where we use the notation

$$\partial_i = \frac{\partial}{\partial x^i}, \quad \dot\partial_\alpha = \frac{\partial}{\partial u^\alpha}, \quad \dot\partial^i_\alpha = \frac{\partial}{\partial u^\alpha_i}, \quad \dot\partial^{ij}_\alpha = \frac{\partial}{\partial u^\alpha_{ij}} \tag{1.1}$$

Let $\mathcal{D}$ be an m-dimensional distribution on K (i.e. an m-dimensional subset of $T(K)$). Let the distribution admit as a basis $\{\mathcal{V}_i\}_{1\le i\le m}$ where the vector fields $\mathcal{V}_i$ take the form

$$\mathcal{V}_i = \partial_i + u^\alpha_i \dot\partial_\alpha + u^\alpha_{ij}\dot\partial^j_\alpha + A^\alpha_{ijk}\dot\partial^{jk}_\alpha\,, \quad 1 \le i \le m \tag{1.2}$$

for some $A^\alpha_{ijk} \in \mathcal{F}(K)$ and where the convention of summation over repeated upper and lower indices is used throughout. The distribution $\mathcal{D}$ is involutive, or completely integrable, if $[\mathcal{D},\mathcal{D}] \in \mathcal{D}$, where $[\cdot,\cdot]$ denotes the Lie brackets. With respect to the basis $\{\mathcal{V}_i\}_{1\le i\le m}$ the involutive condition for the distribution $\mathcal{D}$ is satisfied only if

$$u^\alpha_{ij} = u^\alpha_{ji}\,, \quad A^\alpha_{ijk} = A^\alpha_{jik} = A^\alpha_{jki}\,, \quad \mathcal{V}_i\langle A^\alpha_{jkl}\rangle = \mathcal{V}_j\langle A^\alpha_{ikl}\rangle \tag{1.3}$$

which leads to $[\mathcal{D},\mathcal{D}] = 0$. By the Frobenius theorem we know that if the distribution $\mathcal{D}$ is involutive then through each point $p \in K$ there passes an integral manifold of the same dimension as the distribution $\mathcal{D}$.

Let $\phi : M \to K$ be a smooth (C^∞) map from M to K. The smooth map $\phi : M \to K$ induces the pullback map $\phi^* : \mathcal{F}(K) \to \mathcal{F}(M)$ which maps smooth functions on K to smooth functions on M. We will write $\mathcal{F}(A)$ to mean the set of smooth functions on the manifold A and wherever the map $\phi : M \to K$ has been specified and there is no confusion as to which map we a dealing with we will sometimes use the shorthand notation ${}^*F = \phi^*F = F \circ \phi$ for $F \in \mathcal{F}(K)$.

The smooth map ϕ also induces a smooth differential map ϕ_* such that at each point $p \in M$ the differential map ϕ_* maps members of $T_p(M)$ (the tangent space of M at $p \in M$) to members of $T_{\phi(p)}(K)$ (the tangent space of K at $\phi(p) \in K$). Suppose that (M,ϕ) is an integral manifold of the involutive distribution $\mathcal{D}$ and that at each point $p \in M$ the differential map ϕ_* maps each member of the natural basis of $T_p(M)$ to each member of the basis of $\mathcal{D}$ at $\phi(p) \in (M,\phi)$, i.e. $\phi_*(\partial_i|_p) = \mathcal{V}_i|_{\phi(p)}$. Consider the function $F \in \mathcal{F}(K)$ which upon the action of the pullback of ϕ is mapped to ${}^*F \in \mathcal{F}(M)$. By a straightforward calculation

$$\partial_i({}^*F) = {}^*(\partial_i F) + \frac{\partial\, {}^*u^\alpha}{\partial x^i}\, {}^*(\dot\partial_\alpha F) + \frac{\partial\, {}^*u^\alpha_j}{\partial x^i}\, {}^*(\dot\partial^j_\alpha F) + \frac{\partial\, {}^*u^\alpha_{jk}}{\partial x^i}\, {}^*(\dot\partial^{jk}_\alpha F) \tag{1.4}$$

Since we are using u_i^α and u_{ij}^α as place holders for the first and second partial derivatives of ${}^*u^\alpha$ we immediately write

$$ {}^*u_i^\alpha = \frac{\partial\, {}^*u^\alpha}{\partial x^i}\ , \quad {}^*u_{ij}^\alpha = \frac{\partial\, {}^*u_j^\alpha}{\partial x^i} = \frac{\partial^2\, {}^*u^\alpha}{\partial x^i \partial x^j} \tag{1.5} $$

Because we have no place holders for third partial derivatives and we are confined to K we require that under the action of the pullback of ϕ,

$$ {}^*A_{ijk}^\alpha = \frac{\partial\, {}^*u_{jk}^\alpha}{\partial x^i} = \frac{\partial^3\, {}^*u^\alpha}{\partial x^i \partial x^j \partial x^k} \tag{1.6} $$

In shorthand notation (1.4) can be written

$$ \partial_i({}^*F) = {}^*(\mathcal{V}_i F) \tag{1.7} $$

We shall call a smooth map $\phi : M \to K$ a *regular map* if (M, ϕ) is an m-dimensional integral manifold of the involutive distribution $\mathcal{D}$. The distribution $\mathcal{D}$ will admit as a basis $\{\mathcal{V}_i\}_{1\le i\le m}$, where the vector fields $\mathcal{V}_i$ are given in (1.2). Since $\mathcal{D}$ is involutive we can assume the symmetry relations (1.3). Under the action of the pullback of the map ϕ we have the identities (1.5) and (1.6) which allow us also to apply (1.7). We shall say that the map $\phi : M \to K$ is a *bounded regular map* if it is a regular map and $u^\alpha, u_i^\alpha, u_{ij}^\alpha$ are bounded on the image $\phi(M)$ contained in K.

Consider some N functions $P^\alpha \in \mathcal{F}(K)$ which have the representation given by $P^\alpha(x^i, u^\beta, u_i^\beta, u_{ij}^\beta)$. Suppose that the map $\phi : M \to K$ is associated with an integral manifold of dimension m of the involutive distribution $\mathcal{D}$ such that ϕ annihilates P^α, i.e. $\phi^* P^\alpha = 0$. Then by the pullback identities (1.5) $\phi^* P^\alpha = 0$ has the representation

$$ P^\alpha\left(x^i, {}^*u^\beta, \frac{\partial\, {}^*u^\beta}{\partial x^i}, \frac{\partial^2\, {}^*u^\beta}{\partial x^j \partial x^i}\right) = 0 \tag{1.8} $$

which can be regarded as a system of N PDEs on the base manifold M for the N unknown dependent variables ${}^*u^\alpha \in \mathcal{F}(M)$. On the other hand consider the point set $\Xi \in K$ defined by $\Xi = \{p \in K : P^\alpha = 0\}$. The image $\phi(M)$ will be contained in Ξ and existence theorems for solutions can then be transferred to the study of the properties of the constraints $P^\alpha = 0$ on the point set Ξ. Crucial to this endeavour is the establishment of the symmetry conditions (1.3) on the image $\phi(M)$ contained in the point set Ξ.

The question of existence of solutions to PDEs is often attacked by way of the so called fundamental ideal which contains the contact ideal as a subideal (see for instance [1], [2]). It turns out that $\{\mathcal{V}_i\}_{1\le i\le m}$ forms a basis for the m-dimensional module of Cartan annihilators of the closed contact ideal. In [2] yet another ideal is constructed called the horizontal ideal which contains the contact ideal as a subideal. The set of all solution maps of the horizontal ideal contains all the solution maps of the closed contact ideal. It is shown that the module of Cauchy characteristics of the horizontal ideal admits as a basis $\{\mathcal{V}_i\}_{1\le i\le m}$ and that the horizontal ideal is stable under the Lie transport with respect to the vector fields $\mathcal{V}_i$. It follows that the closure of the horizontal ideal (integrability condition) is gauranteed by the symmetry relations (1.3).

It is worth noting that the analysis that follows can be recast on a setting of the first order contact manifold. To do this one needs to define solution maps as annihilators of the so called balance ideal whose generators consist of the generators of the horizontal ideal and the balance m-forms associated with the PDEs under consideration [2]. Our objectives here are not concerned with establishing existence theorems for PDEs but rather to derive certain results for filtered variables of nonlinear PDEs using space/time/scale as a base manifold. For this purpose the concept of integral manifolds in relation to involutive distributions will be adequate. In the most part we will examine the properties of solution maps that we know exist and in particular solution maps associated with the heat equation. We do this because the heat equation recast on space/scale rather than space/time can be directly linked to spatial filters of the fully resolved variables.

2. Macroscopic Equations

We set $N = 2N'$ and decompose each of u^α, u^α_i and u^α_{ij} into two parts

$$\begin{aligned} &u^A = v^A, \quad u^{N'+A} = r^A, \quad 1 \le A \le N' \\ &u^A_i = v^A_i, \quad u^{N'+A}_i = r^A_i, \quad 1 \le A \le N',\ 1 \le i \le n+2 \\ &u^A_{ij} = v^A_{ij}, \quad u^{N'+A}_{ij} = r^A_{ij}, \quad 1 \le A \le N',\ 1 \le i,j \le n+2 \end{aligned} \tag{2.1}$$

where the v^A will be associated with place holders for the filtered variables and the r^A will be associated with place holders for the residuals which will be defined below. In expanded form the coordinates of K become

$$(x^i, u^\alpha_i, u^\alpha_{ij}) = (x^i, v^A, r^A, v^A_i, r^A_i, v^A_{ij}, r^A_{ij}) \tag{2.2}$$

Throughout, unless otherwise stated, we use the Latin indices for the range $1 \le i,j,k \le m = n+2$, the Greek indices for the range $1 \le \alpha, \beta, \gamma \le N = 2N'$ and the capital Latin indices for the range $1 \le A, B, C \le N'$. For easier identification of certain important operators we use the indices t instead of $n+1$ and η instead of $n+2$, e.g. we write $\mathcal{V}_t$ instead of $\mathcal{V}_{n+1}$ and $\mathcal{V}_\eta$ instead of $\mathcal{V}_{n+2}$.

Let P^A, $(1 \le A \le N')$, have the representation $P^A = P^A(x^i, v^B, v^B_i, v^B_{ij})$ indicating that P^A will be independent of the residuals and their partial derivatives. Suppose that under the pullback of some regular map $\phi : M \to K$, there exists a limiting solution $\phi^* v^A|_{\eta=0^+} = \widetilde{v}^A$, $\widetilde{v}^A \in \mathcal{F}(\mathbb{R}^n \times (0, t_0))$, such that

$$P^A\left(x^i, \widetilde{v}^B, \frac{\partial \widetilde{v}^B}{\partial x^i}, \frac{\partial^2 \widetilde{v}^B}{\partial x^i \partial x^j}\right) = 0 \tag{2.3}$$

We define (2.3) as the system of PDEs which define the fully resolved system and can be represented as the limiting system $\phi^* P^A|_{\eta=0^+} = 0$. Note that given our agreed range of the Latin indices that (2.3) will contain terms involving $\partial/\partial\eta$. In most cases of interest such terms will be redundant. Since these terms will not effect the calculations in the derivations we leave the general representation of P^A as it is to avoid introducing more notation.

Let $\triangle$ denote the spatial Laplacian operator acting on members of $\mathcal{F}(M)$

$$\triangle = \sum_{b=1}^{n} \frac{\partial^2}{\partial x^b \partial x^b} \tag{2.4}$$

and the associated operator acting on members of $\mathcal{F}(K)$

$$\mathcal{L} = \sum_{b=1}^{n} \mathcal{V}_b \mathcal{V}_b \tag{2.5}$$

We shall make repeated use of the vector field

$$\mathcal{W} = \partial_\eta + (\mathcal{L}u^\alpha)\dot{\partial}_\alpha + (\mathcal{L}u^\alpha_i)\dot{\partial}^i_\alpha + (\mathcal{L}u^\alpha_{ij})\dot{\partial}^{ij}_\alpha \tag{2.6}$$

where the convention of summation over repeated upper and lower indices of α and i, j is maintained.

Henceforth, all variables are to be regarded as nondimensional through some appropriate scaling and we shall assume, without further mention, that for any bounded regular map $\phi : M \to K$, boundedness includes the auxiliary condition such that on the image $\phi(M)$ in K we have $\lim_{|x|\to\infty} u^\alpha_i, u^\alpha_{ij}, A^\alpha_{ijk} = 0$. Although in some cases we need only $\lim_{|x|\to\infty} u^\alpha_b = 0$ $(b = 1, \dots, n)$, we do this because we wish, on occasion, to make use of certain fundamental solutions of the heat equation which, under this auxiliary condition in combination with suitable Cauchy data, will gaurantee that they are uniquely defined.

Consider $\phi : M \to K$ to be a bounded regular map that annihilates the N' functions $F^A \in \mathcal{F}(K)$ given by

$$F^A = v^A_\eta - \sum_{b=1}^{n} v^A_{bb} \tag{2.7}$$

Under the action of the pullback of ϕ we have

$$\frac{\partial\, {}^*v^A}{\partial\eta} - \triangle\, {}^*v^A = 0 \quad \text{on } M \tag{2.8}$$

where ${}^*v^A = \phi^* v^A$. Suppose also that

$${}^*v^A|_{\eta=0^+} = \widetilde{v}^A \quad \text{on } \mathbb{R}^n \times (0, t_0) \tag{2.9}$$

for some bounded $\widetilde{v}^A \in \mathcal{F}(\mathbb{R}^n \times (0, t_0))$. The system (2.8) and (2.9) defines a Cauchy problem for the heat equation on space/scale $\mathbb{R}^n \times (0, \eta_0)$ whose coordinates are (x, η) and where the time $t \in (0, t_0)$ enters the problem only as a parameter. Along with the requirement of the boundedness of ϕ and its auxiliary condition, for each $t \in (0, t_0)$ the unique solution ${}^*v^A$ of (2.8) and (2.9) can be written

$${}^*v^A(x, t, \eta) = \int_{\mathbb{R}^n} G(x - x', \eta)\widetilde{v}^A(x', t)\, d^n x' \tag{2.10}$$

where

$$G(x, \eta) = (4\pi\eta)^{-n/2} \exp[-|x|^2/(4\eta)] \tag{2.11}$$

is given in normalized form such that

$$\int_{\mathbb{R}^n} G(x, \eta)\, d^n x = 1\ . \tag{2.12}$$

We use the the notation $d^n x = dx^1 \dots dx^n$. The solution map of (2.7) along with the Cauchy data (2.9) and the boundedness of ϕ defines each ${}^*v^A$ as the spatial Gaussian filter of each $\widetilde{v}^A$. The scale parameter η can be expressed as

$$\eta = \beta\delta^2 \tag{2.13}$$

where δ is a (nondimensional) characteristic space scale associated with the resolution and β is a parameter that controls the rate of damping of the filter.

Suppose that for the filter map ϕ defined above, $(\widetilde{v}^A)$ turns out to be a limiting solution of the system $\phi^* P^A|_{\eta=0^+} = 0$, which has the representation given by (2.3). The N' equations $\phi^* P^A|_{\eta=0^+} = 0$ define the fully resolved system of PDEs which is of interest to us if it generates solutions $(\widetilde{v}^A)$ that are highly fluctuating on

$\mathbb{R}^n \times (0, t_0)$. We cannot in general expect that ${}^*P^A = P^A(x^i, {}^*v^B, {}^*v_i^B, {}^*v_{ij}^B)$ will vanish everywhere on M. We therefore introduce the residuals ${}^*r^A$ that quantify the deviation from zero of $\phi^* P^A$ when $\eta > 0$. The following defines the consistency condition from which immediately follow the exact macroscopic equations that are satisfied by the filtered variables and the exact residuals.

Theorem 2.1 (Consistency)**.** *Let $P^A \in \mathcal{F}(K)$ have the representation $P^A = P^A(x^i, v^B, v_i^B, v_{ij}^B)$ and suppose that there exist $\widetilde{v}^A \in \mathcal{F}(\mathbb{R}^n \times (0, t_0))$, bounded on $\mathbb{R}^n \times (0, t_0)$, such that*

$$P^A\left(x^i, \widetilde{v}^B, \frac{\partial \widetilde{v}^B}{\partial x^i}, \frac{\partial^2 \widetilde{v}^B}{\partial x^i \partial x^j}\right) = 0 \tag{2.14}$$

Let $F^A \in \mathcal{F}(K)$ be given by $F^A = v_\eta^A - \sum_{b=1}^n v_{bb}^A$ and let $\phi : M \to K$ be a bounded regular map such that

$${}^*F^A = 0 \quad \text{on } M \ , \qquad {}^*v^A|_{\eta=0^+} = \widetilde{v}^A \quad \text{on } \mathbb{R}^n \times (0, t_0)\ . \tag{2.15}$$

Let $E^A \in \mathcal{F}(K)$ be defined by

$$E^A = r_\eta^A - \sum_{b=1}^n r_{bb}^A - S^A \tag{2.16}$$

where $S^A \in \mathcal{F}(K)$ is given by

$$S^A = (\mathcal{L} - \mathcal{W}) P^A(x^i, v^B, v_i^B, v_{ij}^B)\ . \tag{2.17}$$

and suppose that in addition ${}^*r^A|_{\eta=0^+} = 0$. Then on M

$$P^A\left(x^i, {}^*v^B, \frac{\partial\, {}^*v^B}{\partial x^i}, \frac{\partial^2\, {}^*v^B}{\partial x^i \partial x^j}\right) + {}^*r^A = \int_0^\eta \int_{\mathbb{R}^n} G(x-x', \eta-\eta')\, {}^*E^A(x', t, \eta')\, d^n x'\, d\eta' \tag{2.18}$$

and hence

$$\left| P^A\left(x^i, {}^*v^B, \frac{\partial\, {}^*v^B}{\partial x^i}, \frac{\partial^2\, {}^*v^B}{\partial x^i \partial x^j}\right) + {}^*r^A \right| \le \eta \sup_{x \in \mathbb{R}^n,\, \eta \in (0, \eta_0)} |{}^*E^A| \tag{2.19}$$

Proof. The system (2.15) defines the Cauchy problem for the heat equation on space/scale $\mathbb{R}^n \times (0, \eta_0)$ whose coordinates are (x, η) and where the time $t \in (0, t_0)$ appears only as a parameter. Given the existence of $\widetilde{v}^A \in \mathcal{F}(\mathbb{R}^n \times (0, t_0))$, bounded on $\mathbb{R}^n \times (0, t_0)$, we are guaranteed that a bounded regular solution map $\phi : M \to K$ associated with (2.15) exists and that $({}^*v^A)$ is unique. We also know that each ${}^*v^A$ is explicitly given by (2.10) and hence defines ${}^*v^A$ as the spatial Gaussian filter of $\widetilde{v}^A$. We note that the regular map $\phi : M \to K$ itself is not unique because it does not as yet place any constraints on the coordinate components r^A, r_i^A, r_{ij}^A of K other than through the pullback identities (1.5), (1.6) and the associated involutive conditions on the distribution $\mathcal{D}$ (1.3).

Consider the point set $\Xi = \{p \in K : F^A = 0\}$. The map $\phi : M \to K$ will map M to $(n+2)$-dimensional integral manifolds of the distribution $\mathcal{D}$ on K contained in the point set Ξ. We have on K

$$\begin{aligned} E^A &= r^A_\eta - \sum_{b=1}^{n} r^A_{bb} - S^A \\ &= (\mathcal{V}_\eta - \mathcal{L})r^A - (\mathcal{L} - \mathcal{W})P^A \\ &= (\mathcal{V}_\eta - \mathcal{L})(P^A + r^A) - (\mathcal{V}_\eta - \mathcal{W})P^A \end{aligned} \tag{2.20}$$

On Ξ we can set $\mathcal{V}_\eta = \mathcal{W}$ and hence (2.20) reduces to

$$(\mathcal{V}_\eta - \mathcal{L})(P^A + r^A) = E^A \quad \text{on } \Xi \tag{2.21}$$

Introducing $Z^A \in \mathcal{F}(K)$ such that $Z^A = P^A + r^A$ it follows that under the action of the pullback of ϕ, (2.21) becomes

$$\frac{\partial\, {}^*Z^A}{\partial \eta} - \triangle\, {}^*Z^A = {}^*E^A \quad \text{on } M \tag{2.22}$$

Since $\phi^* P^A|_{\eta=0^+} = 0$ and ${}^*r^A|_{\eta=0^+} = 0$ we also have

$${}^*Z^A|_{\eta=0^+} = 0 \quad \text{on } \mathbb{R}^n \times (0, t_0) \tag{2.23}$$

The system (2.22), (2.23) defines a Cauchy problem for the nonhomogeneous heat equation on space/scale $\mathbb{R}^n \times (0, \eta_0)$ whose coordinates are (x, η) and where the time $t \in (0, t_0)$ enters the problem only as a parameter. Given that ϕ is a bounded regular map we can write the solution of (2.22) and (2.23) as [8]

$${}^*Z^A(x, t, \eta) = \int_0^\eta \int_{\mathbb{R}^n} G(x - x', \eta - \eta')\, {}^*E^A(x', t, \eta')\, d^n x'\, d\eta' \tag{2.24}$$

where $G(x, \eta)$ is defined by (2.11). This is the identity (2.18). It follows that

$$\begin{aligned} |{}^*Z^A| &= \Big| \int_0^\eta \int_{\mathbb{R}^n} G(x - x', \eta - \eta')\, {}^*E^A(x', t, \eta')\, d^n x'\, d\eta' \Big| \\ &\le \int_0^\eta \int_{\mathbb{R}^n} G(x - x', \eta - \eta') |{}^*E^A(x', t, \eta')|\, d^n x'\, d\eta' \\ &\le \Big(\sup_{x \in \mathbb{R}^n,\, \eta \in (0, \eta_0)} |{}^*E^A| \Big) \int_0^\eta \int_{\mathbb{R}^n} G(x - x', \eta - \eta')\, d^n x'\, d\eta' \end{aligned} \tag{2.25}$$

and the inequality (2.19) follows from (2.12) $\square$

The choice of r^A that renders $E^A = 0$ on the point set Ξ leads us to the exact macroscopic equations that are satisfied by the filtered variables ${}^*v^A$ and the exact residuals ${}^*r^A$:

$$P^A \left(x^i, {}^*v^B, \frac{\partial\, {}^*v^B}{\partial x^i}, \frac{\partial^2\, {}^*v^B}{\partial x^i \partial x^j} \right) + {}^*r^A = 0 \quad \text{on } M \tag{2.26}$$

$$\frac{\partial\, {}^*r^A}{\partial \eta} - \triangle\, {}^*r^A = {}^*S^A \quad \text{on } M \tag{2.27}$$

$${}^*r^A|_{\eta=0+} = 0 \quad \text{on } \mathbb{R}^n \times (0, t_0) \tag{2.28}$$

where $S^A \in \mathcal{F}(K)$ is given by

$$S^A = (\mathcal{L} - \mathcal{W}) P^A(x^i, v^B, v^B_i, v^B_{ij}) \,. \tag{2.29}$$

The fully resolved variables are not explicitly contained in the macroscopic equations but are implied as a limiting solution of (2.26) as $\eta \to 0^+$. As a result the macroscopic system (2.26), (2.27) and (2.28), along with the identity (2.29), have certain useful properties for the purposes of application. In practical application we wish to generate solutions of the filtered variables only on a single scale slice $M_{\eta=\text{const}}$ without the need to access the fully resolved variables. The presence of the term $\partial_\eta {}^*r^A$ in (2.27) is the only remaining obstacle to reach this objective. To overcome this obstacle we resort to approximation methods.

3. Approximation of the Residual

As before consider the point set $\Xi = \{p \in K : F^A = 0\}$ and let $\phi : M \to K$ be the bounded regular map defined in the consistency theorem. Since ϕ is regular it will map M to $(n+2)$-dimensional integral manifolds of the distribution $\mathcal{D}$ on K contained in the point set Ξ. As mentioned in the proof of the the consistency theorem, ϕ is not unique because it does not as yet place any constraints on the coordinate components r^A, r_i^A, r_{ij}^A of K other than through the pullback identities (1.5), (1.6) and the associated involutive conditions on the distribution $\mathcal{D}$ (1.3). Consider the point set $\Xi' \subset \Xi$ such that $\Xi' = \{p \in \Xi : r^A - \eta\mathcal{L}r^A - \eta S^A = 0\}$. Under the action of the pullback of ϕ to the constraints $r^A - \eta\mathcal{L}r^A - \eta S^A = 0$ on Ξ' we have

$$\triangle {}^*r^A - \frac{{}^*r^A}{\eta} + {}^*S^A = 0 \quad \text{on } M \tag{3.1}$$

Under the definition of $E^A \in \mathcal{F}(K)$ given by (2.16) we obtain

$$E^A = r_\eta^A - \frac{r^A}{\eta} \quad \text{on } \Xi' \tag{3.2}$$

Noting that with the additional constraint on ϕ which requires that ${}^*r^A|_{\eta=0^+} = 0$, under the action of the pullback of ϕ (3.2) becomes

$${}^*E^A = \frac{\partial\, {}^*r^A}{\partial\eta} - \frac{{}^*r^A}{\eta} = \frac{\partial\, {}^*r^A}{\partial\eta} - \frac{{}^*r^A - {}^*r^A|_{\eta=0^+}}{\eta} = \frac{\eta}{2}\left[\frac{\partial^2\, {}^*r^A}{\partial\eta^2}\right]_{\eta\in(0,\eta_0)} \tag{3.3}$$

Hence

$$|{}^*E^A| \le \frac{\eta}{2} \sup_{\eta\in(0,\eta_0)} |{}^*r_{\eta\eta}^A| \tag{3.4}$$

Since ϕ is a bounded regular map, as defined in the Section 1, it follows from the consistency theorem that there is a constant $C > 0$ such that

$$|P^A\left(x^i, {}^*v^B, \frac{\partial\, {}^*v^B}{\partial x^i}, \frac{\partial^2\, {}^*v^B}{\partial x^i \partial x^j}\right) + {}^*r^A| \le C\eta^2 \tag{3.5}$$

This demonstrates that for the residual approximation based on (3.1) the exact filtered variables will satisfy the macroscopic system of PDEs (2.26) to a consistency error $O(\eta^2)$. On the other hand if we force (2.26) using a residual that is not exact (i.e. not satisfying (2.27) and (2.28)) we cannot expect that ϕ will be the filter map associated with (2.15).

Let $\widehat{\phi} : M \to K$ be a bounded regular map such that

$$P^A\left(x^i, {}^*\widehat{v}^B, \frac{\partial\, {}^*\widehat{v}^B}{\partial x^i}, \frac{\partial^2\, {}^*\widehat{v}^B}{\partial x^i \partial x^j}\right) + {}^*\widehat{r}^A = 0 \quad \text{on } M\ , \tag{3.6}$$

where ${}^*\widehat{v}^A = \widehat{\phi}^* v^A$, ${}^*\widehat{r}^A = \widehat{\phi}^* r^A$ and ${}^*\widehat{r}^A$ is an approximation of the exact residual. Suppose that in addition ${}^*\widehat{r}^A|_{\eta=0^+} = 0$ on $\mathbb{R}^n \times (0, t_0)$. The system (3.6) can be thought of as the N' PDEs which generate the N' dependent variables ${}^*\widehat{v}^A$. We note that the ${}^*\widehat{v}^A$ cannot be the exact filters of the of the fully resolved variables $\widetilde{v}^A$, i.e. the map $\widehat{\phi}$ cannot annihilate (2.7), because we have forced (3.6) while using residuals that are not exact. To generate the N' approximations for the residuals for the above approximation

$$\triangle\, {}^*\widehat{r}^A - \frac{{}^*\widehat{r}^A}{\eta} + {}^*\widehat{S}^A = 0 \quad \text{on } M \tag{3.7}$$

where ${}^*\widehat{S}^A = \widehat{\phi}^* S^A$ and

$$S^A = (\mathcal{L} - \mathcal{W})P^A \tag{3.8}$$

We have seen above that with a residual equation error of $O(\eta)$ we obtain a consistency error of $O(\eta^2)$. While ${}^*\widehat{v}^A$ cannot be the exact filters of the of the fully resolved variables $\widetilde{v}^A$ we expect that with a consistency error of $O(\eta^2)$ ${}^*\widehat{v}^A$ will be reasonably good approximations of the exact filtered variables ${}^*v^A$. To obtain an estimate for the error ${}^*\widehat{v}^A - {}^*v^A$ is of course a stronger validation of the residual approximation and is very much related, from a geometrical point of view, to the magnitude of the vector field $\mathcal{V}_\eta - \mathcal{W}$ on the image $\widehat{\phi}(M)$ contained in K. Our main objective here is to demonstrate the usefulness of the consistency error alone to examine certain empirically based residual models. It will be seen that consistency will be adequate for this purpose and the stronger validation by way of the error just mentioned will be presented elsewhere.

4. Application

We consider the equations that describe the motion of an incompressible and inviscid fluid. Because we also wish to examine certain empirical gradient models in the next section, we will augment these equations with an equation that describes the transport of a single conservative solute within the fluid medium. Before proceeding a few points need to be made: Any consideration of the Euler or Navier-Stokes equations in the present context may appear problematic because of the current open question on the existence of regular solutions, particularly in three spatial dimensions. Because of their wide use in modelling of complex flows it seems appropriate that they receive some attention although the motivation for the ideas presented here is much wider. It is important to keep in mind throughout that the restriction $\widetilde{v}^A \in \mathcal{F}(\mathbb{R}^n \times (0, t_0))$ is made for brevity rather than by necessity. If working in the class of smooth solutions is too restrictive the consistency theorem could be modified as follows: We replace $\widetilde{v}^A \in \mathcal{F}(\mathbb{R}^n \times (0, t_0))$ with $\widetilde{v}^A \in L_1^{loc}(\mathbb{R}^n)$ for each $t \in (0, t_0)$ and require that (2.14) be satisfied in a generalized sense (see for instance [3]). The solution of (2.15) will still be given by (2.10) but the Cauchy data condition ${}^*v^A|_{\eta=0^+} = \widetilde{v}^A$ will be satisfied a.e. on $\mathbb{R}^n$ in the limit as $\eta \to 0^+$ for each $t \in (0, t_0)$. The macroscopic system of equations (2.26)-(2.28), along with the identity (2.29) for the source term of the residual equation, will still hold.

Let v^b $(b = 1, \dots, n)$ be the placeholders on K for the n filtered velocity components and $v^{n+1} = p$ be the placeholder on K for the filtered pressure. We set $v^{n+2} = \omega$ to denote the mass fraction of some conservative solute in the fluid medium. Here $N' = n+2$. Define

$$P^a = v_t^a + \sum_{b=1}^n v^b v_b^a + p_a \quad 1 \le a \le n \tag{4.1}$$

$$P^{n+1} = \sum_{b=1}^n v_b^b \tag{4.2}$$

$$P^{n+2} = \omega_t + \sum_{b=1}^n v^b \omega_b \tag{4.3}$$

where we shall use the notation $p_i = v_i^{n+1}$, $p_{ij} = v_{ij}^{n+1}$, $\omega_i = v_i^{n+2}$, and $\omega_{ij} = v_{ij}^{n+2}$. A calculation based on (2.17) and (4.1)-(4.3) yields

$$S^a = 2 \sum_{b,c=1}^n v_c^b v_{bc}^a \quad 1 \le a \le n \tag{4.4}$$

$$S^{n+1} = 0 \tag{4.5}$$

$$S^{n+2} = 2 \sum_{b,c=1}^n v_c^b \omega_{bc} \tag{4.6}$$

We should note the following: For a viscous fluid we would introduce the term $-\sum_{b=1}^n v_{bb}^a / Re$ on the right hand side of (4.1), where Re is the Reynolds number. Similarly we may also include a molecular diffusion term $-\kappa \sum_{b=1}^n \omega_{bb}$ on the right hand side of (4.3), where κ is the molecular diffusion coefficient. Both these terms have no effect on the residual equation source terms and (4.4)-(4.6) will remain unchanged.

Since the source term $S^{n+1} = 0$ on K the residual for the continuity equation will vanish. Under the action of the pullback of $\widehat{\phi}$, the system (3.6) and (3.7) for this application becomes

$$\frac{\partial\, {}^*\widehat{v}^a}{\partial t} + \sum_{b=1}^n {}^*\widehat{v}^b \frac{\partial\, {}^*\widehat{v}^a}{\partial x^b} + \frac{\partial\, {}^*\widehat{p}}{\partial x^a} + {}^*\widehat{r}^a = 0 \quad 1 \le a \le n \tag{4.7}$$

$$\frac{\partial\, {}^*\widehat{v}^b}{\partial x^b} = 0 \tag{4.8}$$

$$\frac{\partial\, {}^*\widehat{\omega}}{\partial t} + \sum_{b=1}^n {}^*\widehat{v}^b \frac{\partial\, {}^*\widehat{\omega}}{\partial x^b} + {}^*\widehat{r}^{n+2} = 0 \tag{4.9}$$

$$\triangle\, {}^*\widehat{r}^a - \frac{{}^*\widehat{r}^a}{\eta} + {}^*\widehat{S}^a = 0 \quad 1 \le a \le n \tag{4.10}$$

$$\triangle\, {}^*\widehat{r}^{n+2} - \frac{{}^*\widehat{r}^{n+2}}{\eta} + {}^*\widehat{S}^{n+2} = 0 \tag{4.11}$$

where

$${}^*\widehat{S}^a = 2 \sum_{b,c=1}^n \frac{\partial}{\partial x^b} \left(\frac{\partial\, {}^*\widehat{v}^b}{\partial x^c} \frac{\partial\, {}^*\widehat{v}^a}{\partial x^c} \right) \quad 1 \le a \le n \tag{4.12}$$

$${}^*\widehat{S}^{n+2} = 2 \sum_{b,c=1}^n \frac{\partial}{\partial x^b} \left(\frac{\partial\, {}^*\widehat{v}^b}{\partial x^c} \frac{\partial\, {}^*\widehat{\omega}}{\partial x^c} \right) \tag{4.13}$$

and use has been made of the form invariance of the continuity equation. Since the system (4.7)-(4.13) contains no terms involving ∂_η and no reference to the fully resolved variables, we can seek a solution on any desired scale slice $M_{\eta=\mathrm{const}}$. The choice of the value of the scale parameter η will be dictated by the level of refinement in the spatial discretization used in the numerical solution scheme. The numerical scheme involves also a temporal discretization of the evolution equations (4.7) and (4.9) from which one obtains an update of the velocities and the solute mass fraction at each timestep. For incompressible flows a staggered grid is often used and the velocities updated along with the pressure using a projection method (see for instance [6]). Within each timestep a finite difference approximation of elliptic equations (4.10) and (4.11) are solved iteratively to obtain an update of the residuals. The procedure is repeated until a desired time is reached.

Numerical experiments have been conducted for applications in fluid mechanics by solving (3.6) and (3.7) on single scale slices using finite difference methods [5]. The computations using this approach are found to be stable despite the complex flow patterns that emerge during the breakdown of hydrodynamic stability. For compressible flows, energy balance studies on numerical solutions based on the system (3.6) and (3.7) indicate the presence of some intrinsic property that conserves the total energy of the fluid system. This is particularly interesting given the evidence that the model accommodates the flow of energy both to and from the smaller scales, i.e. internal energy can flow up from the unresolvable scale into the macroscopic scale where it appears as kinetic energy. It is also observed that numerical solutions generated independently on increasing scale slices result in a corresponding increase in the smoothing of finer scale fluctuations in the complex flow patterns, indicating that filtering is occurring.

5. Empirical Gradient Models

We shall investigate a class of residual models in common use today in the field of fluid mechanics. We consider again the flow of an incompressible and inviscid fluid with a single solute. As such we use the prescription given by (4.1)-(4.3). The identities (4.4)-(4.6) still hold under any residual approximation used.

Empirical gradient models take the form

$$r^a = -\eta\nu\mathcal{L}v^a \quad 1 \le a \le n \tag{5.1}$$

$$r^{n+1} = 0 \tag{5.2}$$

$$r^{n+2} = -\eta\kappa\mathcal{L}\omega \tag{5.3}$$

where $\nu, \kappa \in \mathcal{F}(K)$. The coefficients ν and κ are empirically based and are dependent on constant parameters (assumed to be measurable). In application these residual models are explicitly defined and hence can be inserted directly into the system (4.7) and (4.9). The equations (4.10) and (4.11) are of course not applicable here.

The philosophy behind these models is that large scale fluctuations interact in a diffusion like fashion analagous to those at the molecular level. The residuals (5.1) are meant to capture the turbulence stresses in the fluid and the residual (5.3) is meant to capture the solute dispersion in the turbulent fluid medium. The form invariance of the continuity equation is assumed (note that the form invariance of the continuity equation of the previous section is not assumed but follows immediately from the vanishing of the source term S^{n+1}). A useful coverage on current practices and applications of these type of residual models can be found in [4].

In early applications of these models the coefficients μ and κ were assumed to be constants. Due to their failure to predict observations later variants of these models were proposed such that μ and κ are some functions of the dependent variables. We need not investigate any particular case here because it can be shown by consistency alone that empirical gradient type models are flawed in the general case given above and cannot be regarded as approximations of the residuals in any reasonable sense.

Consider the point set $\Xi = \{p \in K : F^A = 0\}$. The map $\phi : M \to K$ of the consistency theorem will map M to $(n+2)$-dimensional integral manifolds of the distribution $\mathcal{D}$ on K contained in the point set Ξ. On the basis of (5.1)-(5.3) we have on K

$$E^a = -\nu\mathcal{L}v^a - S^a - \eta(\mathcal{V}_\eta - \mathcal{L})(\nu\mathcal{L}v^a) \tag{5.4}$$

$$E^{n+1} = 0 \tag{5.5}$$

$$E^{n+2} = -\kappa\mathcal{L}\omega - S^{n+2} - \eta(\mathcal{V}_\eta - \mathcal{L})(\kappa\mathcal{L}\omega) \tag{5.6}$$

On the point set Ξ, (5.4) and (5.6) can be written

$$E^a = -\nu\mathcal{L}v^a - S^a - \eta(\mathcal{W} - \mathcal{L})(\nu\mathcal{L}v^a) \tag{5.7}$$

$$E^{n+2} = -\kappa\mathcal{L}\omega - S^{n+2} - \eta(\mathcal{W} - \mathcal{L})(\kappa\mathcal{L}\omega) \tag{5.8}$$

where we use the fact that $\mathcal{V}_\eta = \mathcal{W}$ on the point set Ξ. Note that in the case that the coefficients ν and κ are constants the $O(\eta)$ terms vanish under the action of the pullback of ϕ. However, whether they are assumed as constants or not, the troublesome zeroth order terms remain. Noting the identities (4.4) and (4.6) we require that

$$\nu\sum_{b=1}^{n} v^a_{bb} \sim -2\sum_{b,c=1}^{n} v^b_c v^a_{bc} \quad 1 \le a \le n \tag{5.9}$$

$$\kappa\sum_{b=1}^{n} \omega_{bb} \sim -2\sum_{b,c=1}^{n} v^b_c \omega_{bc} \tag{5.10}$$

where we use the symbol $\sim$ to denote equality to within an error $O(\eta)$. We see that there do not exist choices for the coefficients $\nu, \kappa \in \mathcal{F}(K)$ that maintain the diffusion like character of the residuals on which the formulas (5.1) and (5.3) are motivated.

Under the action of the pullback of ϕ, the residual equation error ${}^*E^A = O_s(1)$ with respect to the scale parameter η. It follows from the consistency theorem that we have a consistency error $|{}^*P^A + {}^*r^A| = O_s(\eta)$. Since the magnitudes of the residuals ${}^*r^a$ and ${}^*r^{n+2}$ are $O_s(\eta)$ we can expect that in application there will be some contamination of the proposed residual model (5.1)-(5.3) by unwanted terms. It can also be expected that the free parameters that are often contained in explicit formulas for the coefficients ν and κ are not measurable and any fine tuning of these parameters will not improve the order of magnitude estimate of the consistency error.

Attempts have been made to generalize the empirical gradient models by way of

$$r^a = -\eta \sum_{b,c=1}^{n} \mathcal{V}_b(\nu^{bc}\mathcal{V}_c v^a) \quad 1 \le a \le n \tag{5.11}$$

$$r^{n+2} = -\eta \sum_{b,c=1}^{n} \mathcal{V}_b(\kappa^{bc}\mathcal{V}_c \omega) \tag{5.12}$$

where now $\nu^{bc}, \kappa^{bc} \in \mathcal{F}(K)$ are second order symmetric tensors. Choices of their functional dependence on the filtered variables and their partial derivatives have been tried containing additional free parameters that are adjusted to the specific application being considered. However, repeating the above procedure for these residual models reveals that the only choices that can ensure a consistency error $O(\eta^2)$ are given by

$$\nu^{bc} \sim -2v_c^b \tag{5.13}$$

$$\kappa^{bc} \sim -2v_c^b \tag{5.14}$$

The residual based on (5.11) and (5.13) is well known in large eddy simulation and has been derived by series expansion of the integral representation of the Gaussian filter (2.10). Numerical experiments indicate that this model correlates reasonably well with the fluid turbulence stresses and strains inferred by direct numerical simualtions [7]. Unfortunately, computations of turbulent fluid flows using this residual model are highly unstable and therefore the model is of little use in numerical simulation.

While focus has been given here on spatial Gaussian filters by way of the spatial Laplacian differential operator (2.4), it is important to keep in mind observations made in [7] that the residual models are very much dependent on the type of filter being used. However, there appears no reason why the spatial Laplacian differential operator could not be replaced by any other elliptic operator on space/time. This will widen the range of the type of filters that can be studied by the methods presented here and could include spatial, spacio-temporal or temporal only filters. While for these general elliptic operators explicit representations for the consistency error as in (2.18) may not be possible it can be expected that similar order of magnitude estimates of the form (2.19) can be obtained.

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Addendum posted on July 2, 2007.

Both equations (2.3) and (2.14) are meant to represent the expanded form of the statement $P^A|_{\eta=0^+} = 0$. To avoid confusion (2.3) and (2.14) should be written

$$P^A(x, t, 0, \widehat{v}^B, \frac{\partial \widehat{v}^B}{\partial x^i}, \frac{\partial^2 \widehat{v}^B}{\partial x^i \partial x^j}) = 0.$$

The statement following equation (2.20) should read:
On Ξ we can set $\mathcal{V}_\eta P^A = \mathcal{W} P^A$ and hence (2.20) reduces to ...

The statement following equations (5.7)–(5.8) should read: where we use the fact that $\mathcal{V}_\eta(\nu \mathcal{L} v^a) = \mathcal{W}(\nu \mathcal{L} v^a)$ and $\mathcal{V}_\eta(\kappa \mathcal{L} \omega) = \mathcal{W}(\kappa \mathcal{L} \omega)$ on the point set Ξ.
End of Addendum.

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