PROSPECTS FOR A CENTRAL THEORY OF PARTIAL DIFFERENTIAL EQUATIONS

J. W. NEUBERGER

Three episodes in the history of equation solving are finding roots of polynomials, solution of ordinary differential equations, solution of partial differential equations. The first two episodes went through a number of phases before reaching a rather satisfactory state. That the third episode might develop similarly is the topic of this note.

Roots of Polynomials

The quadratic formula for finding roots to second order polynomials has been known since antiquity. Cardan's formulae for finding roots to third- and fourth-degree polynomials were given long ago. Galois demonstrated the impossibility of extending such formulae to higher-order polynomials. Nevertheless, roots of polynomials eventually became well understood. Key to this understanding is the matter of existence of roots (fundamental theorem of algebra) and the practical computation of roots numerically. A result from [12] illustrates a modern point of view on this subject:

Assume p is a non-constant complex polynomial. Call $z : R \to C$ a trajectory of p if z is continuous, has domain all of R, and satisfies

$$p(z)' = -p(z).$$

We speak of the "Newton vector field" having these trajectories. For a trajectory z of p and $s \in R$, if $p'(z(s)) = 0$ and $p(z(s)) \neq 0$ then

$$\{z(t) : t \leq s\}$$

Date: 5 May 2005.

is called a half-trajectory of p. Denote by M the union of all half-trajectories of p.

Theorem 1.

- *Every member of C belongs to some trajectory of p.*
- *If z is a trajectory of p, then $u = \lim_{t\to\infty} z(t)$ exists and $p(u) = 0$.*
- *Each component of the complement of M contains exactly one root of p.*

A plot of the Newton vector field for p visually picks out good approximations to roots of p since they are the points to which trajectories are converging. Once a point close to a root is identified, ordinary Newton's method can be used to calculate that root with great efficiency. Members of C which terminate half-trajectories are "hyperbolic points", that is, points to which at least two half-trajectories converge and at least two trajectories leave. These can also be identified visually from the Newton vector field plot for p.

Ordinary Differential Equations

Some centuries of effort were spent in finding "closed form" solutions to systems of ordinary differential equations (ODE). Sophus Lie's quest was to find integrating factors for systems of ODE. Lie found many interesting things but he didn't provide the start of a central point of view for ODE. That came with the arrival of existence and uniqueness results. Such results give something about which to establish qualitative properties and for which to calculate numerical approximations. The following is a representative result:

Theorem 2. *Assume $c < d$, W is an open subset of a Banach space X and f is a C^1 function from $(c, d) \times W$ to X. If $(b, w) \in (c, d) \times W$, then there is an open interval S containing b on which there is a unique function u satisfying*

$$u(b) = w,\ u'(t) = f(t, u(t)),\ t \in S.$$

This result and its many generalizations give a point of departure for studying a vast variety of problems in ODE.

Requirements for a Central Theory of PDE

What would make a theory of PDE a worthy companion to the above two developments? Such a theory would provide a general setting for the study of systems of PDE. It would provide a vocabulary for specifying supplementary conditions under which a given system has one and only one solution. Such a theory would have as an integral part a basis for computing approximations to solutions. This last requirement is essentially equivalent to asking for a constructive theory, an algorithmic theory. An attempt is made in what follows to describe a germ of such a theory.

First Some Basic Ingredients

The ideas of gradient, critical point, steepest descent, and Sobolev spaces are recalled here. To simplify the discussion only Hilbert spaces are considered - an unnecessary, but convenient restriction.

Assume H is a Hilbert space and ϕ is a real-valued C^1 function on H. The gradient of ϕ is the function $\nabla\phi$ from H to H such that

$$\phi'(u)h = \langle h, (\nabla\phi)(u)\rangle_H, u, h \in H. \tag{1}$$

Such a function $\nabla\phi$ exists, since $\phi'(u)$, the Fréchet derivative at $u \in H$, is a continuous linear real-valued function on H, that is, a member of the dual space of H, and so has a representation (1). A critical point of ϕ is a member u of H such that

$$\phi'(u)h = 0, \text{for all } h \in H,$$

or what is equivalent, $\nabla\phi(u) = 0$.

Steepest descent for ϕ comes in two varieties: discrete and continuous. Discrete steepest consists of starting with $z_0 \in H$ and attempting to define $z_1, z_2, \ldots$ inductively so that

$$z_k = z_{k-1} - \delta_k(\nabla\phi)(z_{k-1}), k = 1, 2, \ldots$$

where $\delta_k > 0$ is chosen optimally in some sense to minimize

$$\phi(z_{k-1} - \delta_k(\nabla\phi)(z_{k-1})), k = 1, 2, \ldots.$$

A minimum u of ϕ, in many cases a zero of ϕ, is sought as

$$u = \lim_{k\to\infty} z_k.$$

Continuous steepest descent for ϕ consists in attempting to locate a minimum or zero of ϕ as

$$u = \lim_{t\to\infty} z(t),$$

where

$$z(0) = z_0 \in H, z'(t) = -(\nabla\phi)(z(t)), t \geq 0.$$

Now for a quick look at Sobolev spaces for those who might not make their living with these. A general reference for these spaces is [1]. Let's see how one of the simplest Sobolev spaces, $H^{1,2}([0,1])$, may be defined. The elements of $H^{1,2}([0,1])$ are the set of all first terms of the closure Q in $L_2([0,1])^2$ of

$$\{\begin{pmatrix} u \\ u' \end{pmatrix} : u \in C^1([0,1])\}. \tag{2}$$

For $\binom{f}{g} \in Q$, g is denoted by f', thus extending the notion of differentiability in a very convenient way for purposes of differential equations (note that no two members of Q have the same first term). For $f \in H = H^{1,2}([0,1])$,

$$\|f\|_H = (\int_0^1 (f^2 + (f')^2))^{\frac{1}{2}}.$$

Note that it is defined on the whole Hilbert space H. Therefore, with $K = L_2([0,1])$, the associated inner product is

$$\langle f, h\rangle_H = \langle f, h\rangle_K + \langle f', h'\rangle_K, f, h \in H.$$

Since Q is a closed subspace of K^2, there is an orthogonal projection P of K^2 onto Q. To see an important property of this projection, define a derivative operator

$$D : H \to K, Df = f', f \in H.$$

To calculate the Hilbert space adjoint $D^* : K \to H$ of D suppose $g \in K$. Then

$$\langle Df, g\rangle_K = \langle f', g\rangle_K = \langle \begin{pmatrix} f \\ f' \end{pmatrix}, \begin{pmatrix} 0 \\ g \end{pmatrix}\rangle_{K^2} = \langle P\begin{pmatrix} f \\ f' \end{pmatrix}, \begin{pmatrix} 0 \\ g \end{pmatrix}\rangle_{K^2}$$
$$= \langle \begin{pmatrix} f \\ f' \end{pmatrix}, P\begin{pmatrix} 0 \\ g \end{pmatrix}\rangle_{K^2} = \langle f, \pi P\begin{pmatrix} 0 \\ g \end{pmatrix}\rangle_H, f \in H$$

where $\pi\binom{r}{s} = r, (r, s \in K)$. Hence,

$$D^* g = \pi P\begin{pmatrix} 0 \\ g \end{pmatrix}.$$

By contrast, if D is considered to be a closed densely defined linear transformation on K (with domain precisely those elements of K which are also in H), then

$$(3) \qquad D^t g = -Dg, \text{ for all } g \in H, \text{ with } g(0) = 0 = g(1),$$

the conventional adjoint of the derivative operator (again having a dense non-closed domain). It's (loosely speaking) the same transformation: the derivative. Yet having two different norms on the domain makes it have two different adjoints. Being clear about such occurences is helpful in dealing with Sobolev gradients (to be introduced shortly).

Let's do this more generally. Assmue that each of L and K is a Hilbert space, and T is a closed, densely defined linear transformation from L to K. The "graph" of T is

$$G_T = \{\begin{pmatrix} x \\ Tx \end{pmatrix} : x \in \text{ the domain of } T\} \subset L \times K$$

"T is *closed*" means that G_T is a closed subset of $L \times K$, the Hilbert space which is the Cartesian product of L and K. (Anyone who thinks functions are sets of order pairs will want to say that G_T *is* T, but the terminology "graph of T" is very common.) Anyway, the domain of T is made into a Hilbert space H by defining the norm

$$\|x\|_H^2 = (\|x\|_L^2 + \|Tx\|_K^2)^{\frac{1}{2}}, \ x \in D(T).$$

Thus $D(T)$ with the norm $\|\cdot\|_H$ is isometric to G_T with the "graph norm" it has as a subspace of $L \times K$.

A formula of Von Neumann, [19],[15] gives that the orthogonal projection of $L \times K$ onto G_T is

$$\begin{pmatrix} (I + T^tT)^{-1} & T^t(I + TT^t)^{-1} \\ T(I + T^tT)^{-1} & I - (I + TT^t)^{-1} \end{pmatrix}. \tag{4}$$

T^t denotes the adjoint of T as a closed, densely defined linear transformation on K into H. The reader may check that (4) is idempotent, symmetric, fixed on G_T and has range in G_T too. Thus (4) is convicted of being the claimed orthogonal projection.

It is an exercise to use this formula to get a workable expression for the orthogonal projection P in the example in which $K = L_2([0, 1])$, $H = H^{1,2}([0, 1])$. To get more general Sobolev spaces which are also Hilbert spaces, take $K = L_2(\Omega)$ for some region in a Euclidean space, H to be a linear subspace of members of K which have a certain number of appropriate partial derivatives; take Tf to be a list of these partial derivatives of f. Then take $\|f\|_H$ to be the "graph norm" of f in the same manner as above. A gradient is called a Sobolev gradient if it is taken with respect to a Sobolev inner product.

These orthogonal projections are fundamental to the construction of Sobolev gradients in both function space and corresponding finite-dimensional approximations. The self-dual nature of such spaces is systematically used despite the emotional attachment of many to the idea that such self-duality is useless (or worse) in the study of differential equations. A novella could be written on this topic.

Some Zero Finding in Hilbert Space

The problem of solving a system of PDEs can often be recast as the problem of finding a critical point of an appropriate real-valued function ϕ on some Hilbert space H. Many important systems arise naturally in this way. Consider a system which doesn't arise this way. Express the system as the search for zero of a function $F : H \to K$, where K is a second Hilbert space, and assume F is C^1. Define

$$\phi(u) = \|F(u)\|_K^2, \ u \in H. \tag{5}$$

So long as, for $u \in H$, $F'(u)$ has range dense in K, it follows that any critical point of ϕ is a zero of F, for

$$\phi'(u)h = \langle F'(u)h, F(u)\rangle_K, u, h \in H.$$

(5) is called a least squares formulation of the problem of finding $u \in H$ so that $F(u) = 0$.

Thus, PDE solving is, in a very large sense, a matter of critical-point finding. In this note, "critical-point-finding" and "variational method" are two ways of indicating the same thing. Here are some reslts on critical points.

Theorem 3. *Assume ϕ is bounded from below and $\nabla\phi$ is locally lipschitzian. If $x \in H$, there is a unique function $z : [0, \infty) \to H$ such that*

$$z(0) = x, \ z'(t) = -(\nabla\phi)(z(t)), t \geq 0. \tag{6}$$

Moreover

$$\int_0^\infty \|(\nabla\phi)(z)\|^2 < \infty.$$

Theorem 4. *If u is an $\omega-$limit point of a function z as in* (6), *then* $(\nabla\phi)(u) = 0$.

Definition. The statement that a C^1 function $\phi : H \to R$ satisfies a gradient inequality (Łojasiewicz inequality) on a region $\Omega \subset H$ means that there are $c > 0, \ \theta \in (0, 1)$ such that

$$\|(\nabla\phi)(v)\|_H \geq c\phi(v)^\theta, v \in \Omega. \tag{7}$$

Theorem 5. *Under the above conditions on ϕ, if* (7) *holds and z satisfies*

$$z'(t) = -(\nabla\phi)(z(t)), \ z(t) \subset \Omega, t \geq 0, \tag{8}$$

then $u = \lim_{t\to\infty} z(t)$ exists and $(\nabla\phi)(u) = 0$.

In [7] it is shown that (7) holds in finite-dimensional cases in a neighborhood of a zero of ϕ provided ϕ is analytic. A direct generalization to infinite dimensions does not hold (take $T \in L(H, K)$ to be compact and self-adjoint, (H, K infinite-dimensional Hilbert spaces), and define $\phi(x) = \|Tx\|_K^2/2, x \in H$). In [16], this inequality was extended to some infinite-dimensional cases to study asymptotic limits of solutions to time-dependent PDE (see also [2],[5]). Theorem 8 gives a sufficient condition for a gradient inequality to hold.

Theorem 6. *Assume that G is a C^1 function on H and*

$$\phi(x) = \|x\|_H^2/2 + G(x), x \in H.$$

Assume also that ϕ is coercive ($\phi(x) \to \infty$ as $\|x\|_H \to \infty$), and that $\nabla(G)$ is compact (if $\{x_k\}_{k=1}^{\infty}$ is a bounded sequence in H, then $\{\nabla G(x_k)\}_{k=1}^{\infty}$ has a convergent subsequence) and locally lipschitzian. If $z : [0, \infty) \to H$ satisfies (6), then z has an $\omega-$limit point, and each such point is a zero of $\nabla \phi$.

For the next theorem, suppose that K is a second Hilbert space, $F : H \to K$ is C^1,

$$\phi(x) = \|F(x)\|_K^2/2, x \in H, \tag{9}$$

and ϕ has a locally lipschitzian derivative. Note that

$$(\nabla \phi)(x) = F'(x)^* F(x), x \in H \tag{10}$$

where for $x \in H$, $F'(x)^* : K \to H$ is the Hilbert space adjoint of $F'(x)$.

Theorem 7. *In addition to (9), assume that*

$$\|(\nabla \phi)(v)\|_H \geq c\|F(v)\|_K, v \in B_r(x) \tag{11}$$

(i.e., ϕ satisfies (7) with $\theta = \frac{1}{2}$). If

$$\|F(x)\|_K \leq rc,$$

then there is $u \in B_r(0)$ so that

$$F(u) = 0. \tag{12}$$

In the case of Theorem 7, a sufficient condition for the gradient inequality (7) to hold on Ω is the following from [11]:

Theorem 8. *Assume that* $\Omega \subset H$, $F : \Omega \to K$ *is* C^1 *and there are given* $M, b > 0$ *such that if* $g \in K$ *and* $x \in \Omega$, *then there is* $h \in H$ *with* $\|h\|_H \leq M$ *and*

$$\langle F'(x)h, g\rangle_K \geq b\|g\|_K.$$

Then for $c = 2^{-\frac{1}{2}}b/M$,

$$\|(\nabla\phi)(u)\| \geq c\phi(x)^{\frac{1}{2}}, x \in \Omega.$$

Thus a gradient inequality is implied by sufficiently good uniform approximation to members g of K by elements $F'(u)h$. The finding of solutions or approximate solutions h to linear equations of the form

$$F'(u)h = g,$$

where u, g are given, is central to the main point of [9]. I am leading to a recent result which captures much of the spirit of [9], and whose proof is very close to one for a slightly different result in [13]. But first some background.

In addition to more conventional metrics, a gradient can be taken with respect to a Riemannian metric. Assume F is a C^1 function from H to H and $\phi(u) = \|F(u)\|_H^2$, $u \in H$. F induces a Riemannian metric on H by means of, given $u \in H$,

$$\langle x, y\rangle_u = \langle F'(u)x, F'(u)y\rangle_H, x, y \in H. \tag{13}$$

Assuming $F'(u)$ is bounded below for all $u \in H$, a gradient can, given $u \in H$, be defined as g_u such that

$$\phi'(u)h = \langle h, g_u\rangle_u, h \in H.$$

But also then,

$$\phi'(u)h = \langle F'(u)h, F(u)\rangle_H, h \in H.$$

Thus

$$\langle F'(u)h, F(u)\rangle_H = \langle F'(u)h, F'(u)g_u\rangle_H, h \in H,$$

with g_u as in (13), and so $F'(u)g_u = F(u)$. This suggests that the Newton vector field for F belongs to the same family of gradients to which Sobolev gradients belong.

With this motivation here are two more results to add to the above list. The first might be compared with Theorem 7, and is a zero-finding result; the second is a version of the Nash-Moser inverse function theorem. See [13] for arguments. For these two results, assume that each of H, J, K is a Banach space. Assume also that H is compactly embedded in J, in the sense that if $x_1, x_2, \ldots$ is a sequence in H whose terms are uniformly bounded in norm by M, then this sequence has a subsequence convergent in the J topology to an element of H which has H norm not exceeding M. For $x \in H$ and $r > 0, B_{r,H}(x)$ and $b_{r,H}$ denote, respectively, the closed and open balls in H with center x and radius r.

Theorem 9. *Given $x_0 \in H$ and $r > 0$, assume that $F : B_{r,H}(x_0) \to K$ is continuous in the J topology and that if $u \in B_{r,H}(x_0)$ then there is $h \in B_{r,H}(0)$ such that*

$$\lim_{t\to 0+} \frac{1}{t}(F(x+th) - F(x)) = -F(x_0).$$

Then there is $u \in B_{r,H}$ such that $F(u) = 0$.

Closer to Moser's main result in [9] is the following inverse function theorem:

Corollary 1. *Suppose $M > 0$ and $g \in K$. Assume also that $G : B_{r,H}(0) \to K$, with $G(0) = 0$, is continuous in the J topology, and that if $y \in B_{r,H}(0)$ there is $h \in B_{M,H}(0)$ such that*

$$\lim_{t\to 0+} \frac{1}{t}(G(x+th) - G(x)) = g.$$

Then if $0 \le t \le r/M$ there is $u \in B_{r,H}(0)$ such that $G(u) = tg$.

(Just take $F(x) = G(x) - g,\ x \in B_{r,H}$, and apply Theorem 9).

Equation (6) is an ordinary differential equation in infinite dimensions. Solutions to (6) can be tracked numerically to obtain approximations to solutions u to $F(u) = 0$. This gives the prospect of a unified numerical approach to a very large collection of problems in PDE. For problems in the form (9), existence of a solution u to $F(u) = 0$ can be established if a gradient inequality can be shown to hold on a region containing a trajectory z of (6). Establishing a gradient inequality is equivalent, according to Theorem 8, to the uniform boundedness of solutions to a certain collection of linear problems.

Differential Equations: More Concrete Developments

A very simple example illustrates how to deal with equations for which no natural variational principle is in hand. Experience has shown that someone who codes successfully this example is prepared to code much more complicated problems, problems of scientific interest.

Example. Find u in the Sobolev space $H = H^{1,2}([0,1])$ so that

$$u' - u = 0.$$

Define

$$\phi(u) = \frac{1}{2}\int_0^1 (u'-u)^2,\ u \in H. \tag{14}$$

Something that occurs for many systems of differential equations happens in this case: a zero of the corresponding Sobolev gradient $\nabla\phi$ is also a zero of ϕ. Here is a representation of $\nabla\phi$ in the present case.

Define $F : H \to K = L_2([0,1])$ by

$$F(u) = u' - u, \phi(u) = \|F(u)\|_K^2/2, u \in H. \tag{15}$$

Note that

$$\phi'(u)h = \langle h'-h, u'-u\rangle_K = \langle \begin{pmatrix} h \\ h' \end{pmatrix}, \begin{pmatrix} u-u' \\ u'-u \end{pmatrix}\rangle_{K\times K}, u, h \in H. \tag{16}$$

Denote by P the orthogonal projection of $K \times K$ onto Q in (2), and define $\pi : K \times K \to K$ by $\pi\binom{f}{g} = f$. Then from (16)

$$\phi'(u)h = \langle \begin{pmatrix} h \\ h' \end{pmatrix}, P\begin{pmatrix} u-u' \\ u'-u \end{pmatrix}\rangle_{K\times K},$$

and so

$$\phi'(u)h = \langle h, \pi P \begin{pmatrix} u - u' \\ u' - u \end{pmatrix} \rangle_H, h, u \in H;$$

consequently

$$(\nabla\phi)(u) = \pi P \begin{pmatrix} u - u' \\ u' - u \end{pmatrix}, u \in H.$$

A finite-dimensional counterpart, now follows. It is based on the same simple example, but the considerations generalize rather easily.

Pick a positive integer n and divide the interval $[0, 1]$ into n pieces of equal length. Take $\delta = \frac{1}{n}$, and define $D_0, D_1 : R^{n+1} \to R^n$ so that if $u = (u_0, u_1, \ldots, u_n) \in R^{n+1}$ then

$$D_0 u = (\frac{u_1 + u_0}{2}, \ldots, \frac{u_n + u_{n-1}}{2}),$$

$$D_1 u = (\frac{u_1 - u_0}{\delta}, \ldots, \frac{u_n - u_{n-1}}{\delta});$$

take

$$Du = \begin{pmatrix} D_0 u \\ D_1 u \end{pmatrix}.$$

Define a new inner product between elements $u, v \in R^{n+1}$:

$$\langle u, v \rangle_{S,n} = \langle Du, Dv \rangle_{R^{2n}}.$$

Let us call R^{n+1} under this inner product H_n: a discrete version of $H = H^{1,2}$ above. A finite-dimensional version ϕ_n of (14) is given by

$$\phi_n(u) = \|D_1 u - D_0 u\|^2_{R^n}/2, u \in R^{n+1}.$$

Note that for $u, h \in R^{n+1}$,

$$\phi_n'(u)h = \langle D_1 h - D_0 h, D_1 u - D_0 u \rangle_{R^n} = \langle h, (D_1 - D_0)^t (D_1 - D_0) u \rangle_{R^{n+1}},$$

so that

$$(\nabla_n \phi_n)(u) = (D_1 - D_0)^t (D_1 - D_0) u;$$

this is the ordinary gradient of ϕ_n, that is to say, the list of relevant partial derivatives.

Now for $u \in R^{n+1}$, $\phi_n'(u)$ is also a linear functional on H, that is, on R^{n+1} under the norm $\|\cdot\|_{S,n}$. Accordingly there is the function $\nabla_{S,n}\phi_n$ for which

$$\begin{aligned}\phi_n'(u)h = \langle h, (\nabla_{S,n}\phi_n)(u)\rangle_{S,n} &= \langle Dh, D(\nabla_{S,n}\phi_n)(u)\rangle_{R^{2n}} \\ &= \langle h, D^t D(\nabla_{S,n}\phi_n)(u)\rangle_{R^{n+1}}, u, h \in R^{n+1}.\end{aligned}$$

Thus,

$$(D^t D)(\nabla_{S,n}\phi_n)(u) = (\nabla_n \phi_n)(u)$$

and so

$$(\nabla_{S,n}\phi_n)(u) = (D^t D)^{-1}(\nabla_n \phi_n)(u), u \in R^{n+1}.$$

This relationship between ordinary numerical gradient and its Sobolev gradient counterpart is a general phenomenom. A numerical analyst recognizes this Sobolev gradient to be a preconditioned version of the ordinary one. In [4], [11] this statement is reinforced in detail to show that finite-dimensional Sobolev gradient theory gives an organized approach to preconditioning.

This is a place to point out that if in (14) a gradient g in $L_2([0,1])$ were sought in order to represent ϕ', so that

$$(\phi'(u))h = \langle h, g(u)\rangle_{L_2([0,1])}, u, h \in L_2([0,1]),$$

the gradient g would be only densely defined on $L_2([0,1])$ and discontinuous everywhere it is defined. Such an object is not a promising one to approximate numerically. However, the ordinary gradient of ϕ_n is just what one would try to use for such an approximation. Now it is legendary that such ordinary gradients, defined for problems in differential equations, perform very poorly numerically, the performance degenerating dramatically as the number of mesh points increases. By contrast, the Sobolev gradient of ϕ is defined everywhere and is a differentiable function. The Sobolev gradient of ϕ_n performs very nicely numerically: typically the number of iterations required does not depend on the number of mesh points chosen. This is an instance of this writer's First Law of Numerical Analysis:

NUMERICAL DIFFICULTIES AND ANALYTICAL DIFFICULTIES ALWAYS COME IN PAIRS

An orthogonal projection related to the above example is given by

$$P = D(D^tD)^{-1}D^t.$$

It is the orthogonal projection of R^{2n} onto the range of D. It is an exercise to reconcile this expression with (4).

The above is an indication how a variational principle can be established for many systems of differential equations. If a given system corresponds to the Euler-Lagrange functional on a Sobolev space, there is another, direct method available. Examples include energy functionals for Hamiltonians, elasticity, transonic flow, Ginzburg-Landau functionals for superconductivity, oil-water separation problems, minimal surfaces, Yang-Mills functionals. Generally, if an energy functional is available, it is better to look directly for critical points of the functional rather than forming a new functional based on the corresponding Euler-Lagrange equations (for one thing, those are of degree twice the maximum order of derivative appearing in the energy functional).

For an illustration, assume n is a positive integer and Ω is a domain in R^n. Define ϕ by

$$\phi(u) = \int_\Omega (\frac{1}{2}\|\nabla u\|^2_{R^m} + G(u)) \tag{17}$$

for $u \in H$, H being an appropriately chosen Sobolev space, so that $G \in C^1$ and $\nabla\phi$ is locally lipschitzian. Assume also that ϕ is bounded below. Then for $u, h \in H$,

$$\phi'(u)h = \int_\Omega (\langle \nabla h, \nabla u\rangle_{R^n} + G'(u)h) = \langle \begin{pmatrix} h \\ \nabla h \end{pmatrix}, \begin{pmatrix} (\nabla G)(u) \\ \nabla u \end{pmatrix} \rangle_{H\times K}, \tag{18}$$

K being an appropriate L_2 space. Denoting by P the orthogonal projection of $H \times K$ onto

$$\{\begin{pmatrix} v \\ \nabla v \end{pmatrix} : v \in H\},$$

one has

$$\phi'(u)h = \langle h, \pi P\begin{pmatrix}(\nabla G)(u)\\ \nabla u\end{pmatrix}\rangle_H$$

where here π picks out the first component of $P\binom{\nabla G(u)}{\nabla u}$. Thus for a Sobolev gradient of ϕ

$$(\nabla\phi)(u) = \pi P\begin{pmatrix}(\nabla G)(u)\\ \nabla u\end{pmatrix} = u - \pi P\begin{pmatrix}u - \nabla G(u)\\ 0\end{pmatrix},\ u \in H. \tag{19}$$

On bounded regions with a smooth boundary the transformation

$$u \to \pi P\begin{pmatrix}u - (\nabla G)(u)\\ 0\end{pmatrix}$$

(where $\pi\binom{f}{g} = f$) may be seen, by examining the relevant projection P, to be compact.

Furthermore, u is a critical point of ϕ if and only if

$$(\nabla\phi)(u) = 0. \tag{20}$$

The Sobolev gradient equation (20) is a substitute for the corresponding Euler-Lagrange equations together with any "natural" boundary conditions arising from the required integration by parts used in obtaining these equations from ϕ. The functional (17) contains only first derivatives but the corresponding Euler-Lagrange equations require second derivatives. Use of equation (20) avoids the old problem, already noted by Hilbert, of introducing more derivatives than the basic problem presupposes.

The Sobolev gradient is a continuous function whose zeros are critical points of ϕ which may be sought by means of limits at infinity of a solution z to (6). Contrast this with the usual nonconstructive (cf [3],[18]) approach to dealing with (17): defining a minimizing sequence $\{u_k\}_{k=1}^{\infty}$, that is

$$\lim_{n\to\infty} \phi(u_k) = \inf_{u\in H} \phi(u),$$

then attempting to extract a convergent subsequence of this sequence whose limit is a minimum of ϕ and consequently a solution to the corresponding Euler-Lagrange equations. Continuous steepest descent (6) provides a constructive alternative, so it is not surprising that its finite-dimensional versions yield viable numerical methods.

Numerical considerations for directly computing critical points of energy functionals such as (17) are quite similar to those for (9). Sometimes for an energy functional it is helpful to define a second function J:

$$J(u) = \|(\nabla\phi)(u)\|_H^2,\ u \in H$$

and then use ∇J in place of $\nabla\phi$ in (6). This is used when there are saddle points for ϕ for which numerical computations are unstable. Critical points of ϕ become local minima of J. An alternative point of view is found in [10], which gives a way to constrain trajectories in seeking a critical point numerically.

Boundary Conditions

So far little has been said about how these ideas relate to boundary conditions. Following are two rather distinct developments on this topic, both of which contain a guide to numerics.

Traditionally the role of boundary conditions in connection with partial differential equations is to give conditions on boundary values under which a given system has a unique solution. It should be recognized that specifying conditions on a boundary of a region (on which solutions are to be found) is often not known to be adequate for making the solution unique.

Consider for example a Tricomi equation [8], a version of which is the following: Find u on $\Omega = [0, 1] \times [-1, 1]$ so that

$$u_{1,1}(x, y) + yu_{2,2}(x, y) = 0, (x, y) \in \Omega. \tag{21}$$

It my understanding that, after decades of consideration, it is still not known what boundary conditions might be placed on a prospective solution u to (21) in order that there be one and only one solution. A main problem with (21) is that it is elliptic above the real line and hyperbolic below. For elliptic, parabolic, or hyperbolic problems, ideas about boundary conditions are quite well understood. But many systems defy such categorization.

The first of my two comments on the "supplementary condition" problem deals with problems in the form (9) but applies equally to those in the form (17).

Assume each of H, K, S is a Hilbert space, F is a C^1 function from H to K, and B is a C^1 function from H to S.

Typical Problem. Find $u \in H$ so that

$$F(u) = 0, \; B(u) = 0. \tag{22}$$

Think of the first equation in (22) as specifying a system of differential equations and the second equation as supplying supplementary conditions.

Thus if we had the simple example above but with the condition $u(0) = 1$ imposed on a solution u, we would define

$$F(u) = u' - u, \; B(u) = u(0) - 1, u \in H^{1,2}([0,1]). \tag{23}$$

In the general case, take

$$\phi(v) = \|F(v)\|_K^2/2, v \in H, \tag{24}$$

and for each $v \in H$, define

$$H_{B,v} = \{h \in H : B'(v)h = 0\}.$$

For each $v \in H$, define $P_B(v)$ to be the orthogonal projection of H onto $H_{B,v}$. Then

$$\phi\prime(v)h = \langle F'(v)h, F(v)\rangle_K = \langle h, F'(v)^*F(v)\rangle_H = \langle h, P_B(v)F'(v)^*F(v)\rangle_H, v \in H, h \in H_{B,v}$$

so that the corresponding Sobolev gradient is

$$(\nabla_B\phi)(v) = P_B(v)F'(v)^*F(v), v \in H.$$

Suppose $x \in H$ and $B(x) = 0$, and assume that both P_B and $F'(\cdot)^*F(\cdot)$ are C^1. Then there is $z : [0,\infty) \to H$ so that if

$$z(0) = x \in H, z'(t) = -(\nabla_B\phi)(z(t)), t \geq 0,$$

then

$$B(z)'(t) = B'(z(t))z'(t) = -B'(z(t))(\nabla_B\phi)(z(t)) = 0, t \geq 0$$

since

$$(\nabla_B\phi)(z(t)) \in N(B'(z(t)), t \geq 0.$$

Thus continuous steepest descent with this Sobolev gradient, starting at x, preserves the supplementary condition satisfied by the initial condition, i.e.,

$$B(z(t)) = B(x) = 0, t \geq 0$$

and so $B(u) = 0$ if $u = \lim_{t\to\infty} z(t)$.

Here is a second rather general suggestion about the "supplementary condition" problem. I make no attempt for maximum generality; more on this issue can be found in [11] and references therein. Assume H is a Hilbert space, ϕ is a nonnegative C^2 function on H, and $\nabla\phi$ is the Sobolev gradient of ϕ. Then if $x \in H$, there is a unique solution z to

$$z(0) = x \in H,\ z'(t) = -(\nabla\phi)(z(t)), t \geq 0. \tag{25}$$

Assume also that for each such $x \in H$ the corresponding solution z to (25) satisfies

$$u = \lim_{t\to\infty} z(t) \text{ exists,} \tag{26}$$

and consequently u is a critical point of ϕ. Call $w, y \in H$ equivalent provided there is $u \in H$ such that if x is either of w and y, and z satisfies (25), then (26) holds.

This notion of equivalence gives a foliation of H, two members of H being in the same leaf of the foliation if and only if they are equivalent. This leads to a setting in which each leaf of the foliation contains precisely one critical point of ϕ. An analytical, topological, or algebraic (preferably all three) understanding of this foliation tags in a potentially useful way each critical point of ϕ with a leaf of the foliation.

How does this look in a linear case? Assume T is a continuous linear transformation from a Hilbert space H to the Hilbert space

K. Define $\phi : H \to K$ by

$$\phi(x) = \|Tx\|_K^2/2,\ x \in H.$$

Then

$$\phi'(x)h = \langle Th, Tx\rangle_K = \langle h, T^*Tx\rangle_H$$

so that

$$(\nabla\phi)(x) = T^*Tx,\ x \in H.$$

Pick $x \in H$ and consider z satisfying (25). Note that not only does

$$u = \lim_{t\to\infty} z(t) \text{ exist,}$$

but u is the nearest zero of T to the initial value x. An understanding of the resulting foliation would give a hold on the set of all solutions to (21).

Numerical Approximations

Quite a number of numerical implementations have been worked out for Sobolev gradients. The Ginzburg-Landau development for superconductivity is chosen as a representative application. Work described is that of the present author and his long-time collaborator R.J. Renka (see [14] and references therein). The Ginzburg-Landau functional ϕ used is based on a region Ω, chosen here to be a subset of R^2 although similar considerations hold in R^3. Take $H = H^{1,2}(\Omega, C) \times H^{1,2}(\Omega, R^2)$ and $\phi : H \to R$ defined by

(27)

$$\phi(u, A) = \int_\Omega (\|\nabla u - iuA\|^2 + \|\nabla\times A - H_0\|^2 + \frac{\kappa^2}{4}(|u|^2-1)^2), (u, A) \in H,$$

where H_0 is a given C^1 function on Ω. The complex-valued function u is an “order parameter”, meaning here that $|u|^2$ indicates density of superconducting electrons. The function $\nabla \times A$ is an induced magnetic field, and H_0 an imposed magnetic field.

A Sobolev gradient for ϕ is constructed along the lines of the simple example. The figures gives some representative results. In each of these figures, the magnitude of the magnetic field $\nabla \times A$

corresponding to a critical point of (27) is depicted. In the first figure, the “flippers” of the squid-like hole are shorter than corresponding flippers in the second figure. In the first figure, there is a ”free” vortex, one not pinned by a given structure, whereas in the second figure there is no such free vortex. These pictures illustrate how small changes in a superconducting device may lead to substantially different critical points. These pictures, from a code by Robert Renka, were obtained by Barbara Neuberger as part of a program seeking to aid design of superconductors by means of simulations. For purposes of superconducting electronics, one wants to understand how to place holes or moats which will attract vortices in order to leave substantial parts of the device free of vortices, places in which it is attractive to put superconducting circuits. A recent reference for this program is [14]. Other applications are [17], [11] and references therein. These other applications include transonic flow problems and elasticity problems as well as a variety of Ginzburg-Landau type problems. Yang-Mills [6] functionals are very close in structure to those of the Ginzburg-Landau functional of superconductivity. It is an interesting research problem to code the Yang-Mills functionals using Sobolev gradients.

A principal interest of this writer in these applications of Sobolev gradients is that they look like developments moving in the direction of a central theory of partial differential equations. Sobolev gradients have worked in all known instances in which they have been seriously tried.

Conclusion

The sketch above seeks to place a broad part of PDE into a variational setting, a setting which includes both numerical and theoretical considerations. A key element is the systematic use of self-duality of the Sobolev spaces involved. It is briefly indicated how a wide variety of boundary conditions (more accurately, supplementary conditions) may be dealt with in a systematic way.

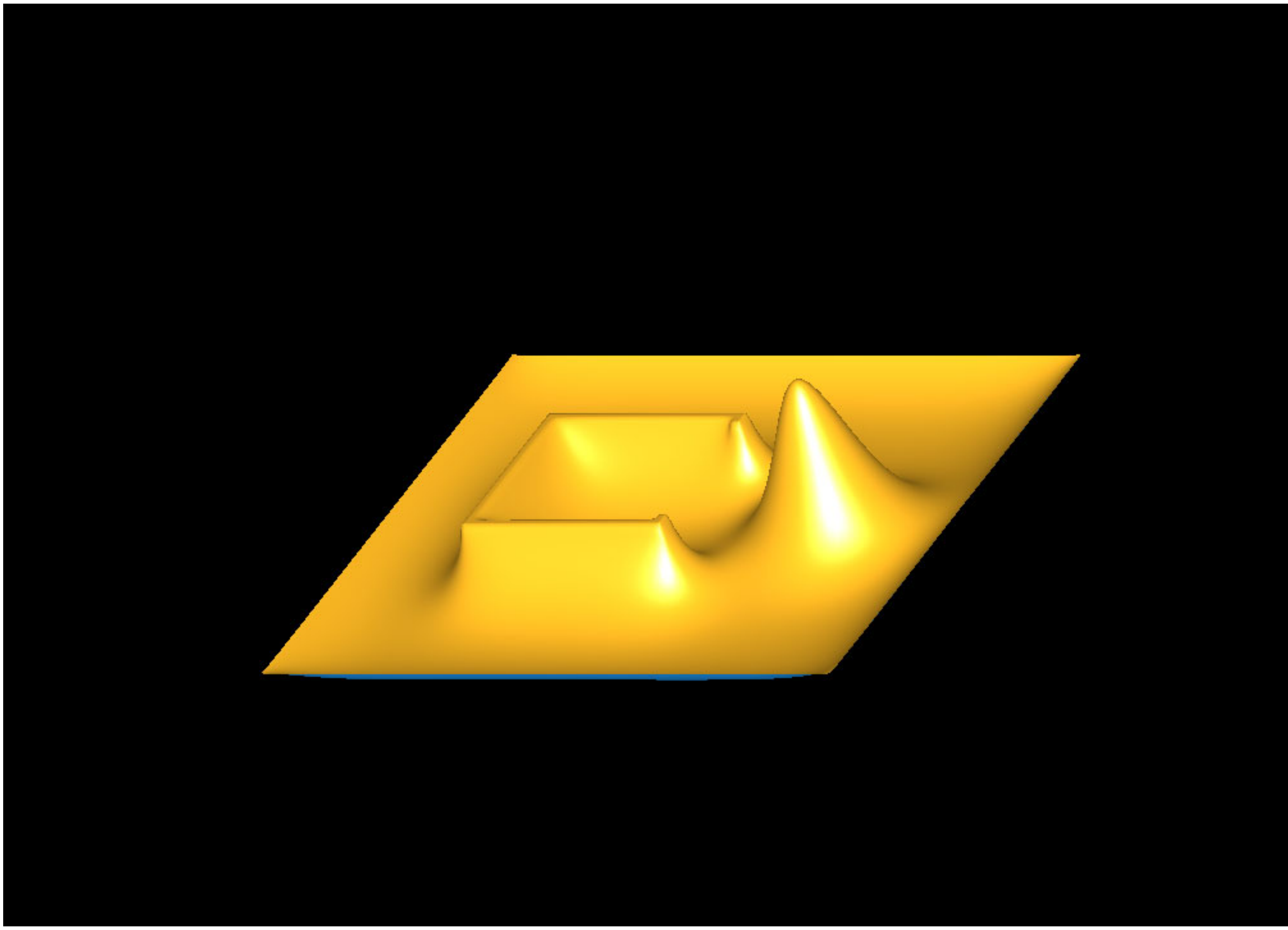

Figure 1. Magnetic Field on a Squid with Smaller Flippers

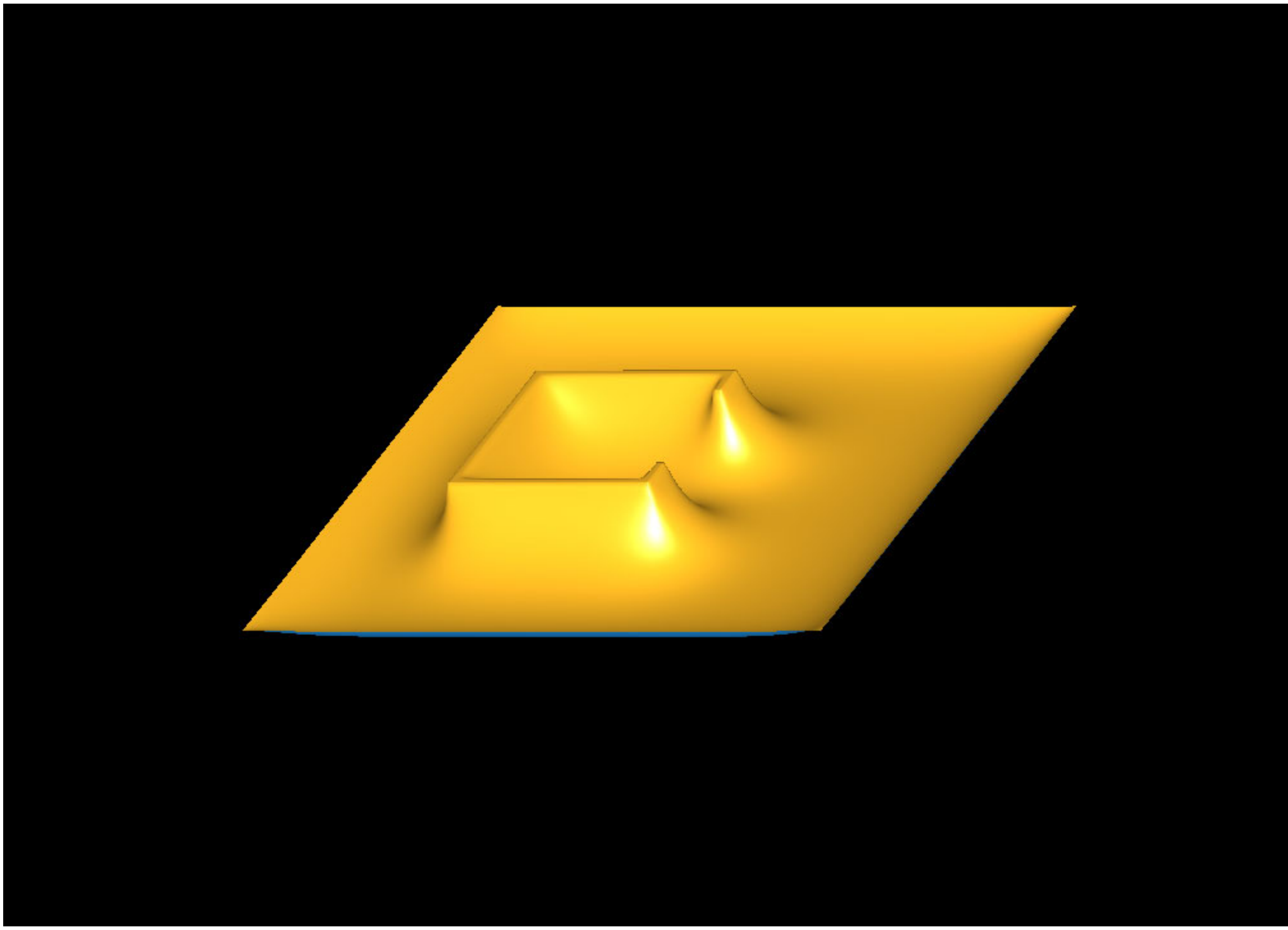

Figure 2. Magnetic Field on a Squid with Longer Flippers

References

[1] R.A. Adams, *Sobolev Spaces*, Academic Press, 1978.

[2] R. Chill and M. A. Jendoubi, *Convergence to steady states in asymptotically autonomous semilinear evolution equations*, Nonlinear Analysis 53 (2003), 1017-1039.

[3] L.C. Evans, *Weak Convergence Methods for Nonlinear Partial Differential Equations*, CBMS Reg. Conf. Ser., Amer. Math. Soc. 1990

[4] Faragó, I., Karátson, J., *Numerical solution of nonlinear elliptic problems via preconditioning operators: Theory and applications.* Advances in Computation, Volume 11, NOVA Science Publishers, New York, 2002.

[5] S.-Z. Huang and P. Takač, Convergence in gradient-like systems which are asymptotically autonomous and analytic, Nonlinear Anal. 46 (2001), 675-698.

[6] A. Jaffe and C. Taubes *Vortices and Monopoles. Structure of Static Gauge Theories*, Progress in Physics 2, 1980.

[7] S. Łojasiewicz, Une propriété topologique des sous-ensembles analytiques rés, Colloques internationaux du C.N.R.S.: Les équations aux dérivées partielles, Editions du C.N.R.S., Paris (1963), 87-89.

[8] D. Lupo and K.R. Payne, *On the maximum principle for generalized solutions to the Tricomi problem*, Commun. Contemp. Math. 2 (2000), 535-557.

[9] J. Moser, *A Rapidly Convergent Iteration Method and Non-Linear Differential Equations*, Ann. Scuola Normal Sup. Pisa, 20 (1966), 265-315.

[10] John M. Neuberger, *A numerical method for finding sign changing solutions of superlinear Dirichlet problems*, Nonlinear World 4 (1997), 73-83.

[11] J.W. Neuberger, *Sobolev Gradients and Differential Equations*, Springer Lecture Notes in Mathematics 1670, 1997.

[12] J.W. Neuberger, *Continuous Newton's Method for Polynomials*, Mathematical Intelligencer, 21 (1999), 18-23.

[13] J.W. Neuberger, *A near minimal hypothesis Nash-Moser Theorem*, Int. J. Pure. Appl. Math.. 4 (2003), 269-280.

[14] J. W. Neuberger and R. J. Renka, *Numerical determination of vortices in superconductors: simulation of cooling*, Supercond. Sci. Technol 16 (2003), 1-4.

[15] B. Sz.-Nagy and F. Reisz, *Functional Analysis*, Ungar, 1955.

[16] L. Simon, *Asymptotics for a class of non-linear evolution equations with applications to geometric problems*, Ann. Math. 118 (1983), 525-571.

[17] S. Sial, J. Neuberger, T. Lookman, A. Saxena, *Energy minimization using Sobolev gradients: applications to phase separation and ordering.*, J. Comp. Physics 189 (2003),88-97.

[18] M. Struwe, *Variational Methods*, Ergebnisse Mathematik Grenz., Springer, 1996.

[19] J. von Neumann, *Functional Operators II*, Annls. Math. Stud. 22, (1940).

[20] E. Zeidler, *Nonlinear Functional Analysis and its Applications III*, Springer-Verlag, 1985.

E-mail address: jwn@unt.edu

Department of Mathematics, University of North Texas, Denton, TX 76203-1430