Mathematical Metaphors: Initial Problem Statement Formulation and Transformation to a Solvable Representation

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Abstract

This paper addresses the critical issue of the development of intelligent or assisting tools for the scientist who is working in the initial problem formulation and mathematical model representation stage of research. In particular, examples of that representation in fluid dynamics and instability theory are discussed. The creation of a mathematical model that is ready for application of certain solution strategies requires extensive symbolic manipulation of the original mathematical model. These manipulations can be as simple as term reordering or as complicated as discovery of various symmetry groups embodied in the equations, whereby Backlund-type transformations create new determining equations and integrability conditions or create differential Grobner bases that are then solved in place of the original nonlinear PDEs. Here I discuss several examples of the kinds of problem formulations and transforms that can be frequently encountered in model representation for fluids problems. The capability of intelligently automating these types of transforms is advocated.

Introduction

There are several stages of activity involved in computational science. The first of these begins with the scientist finding and expressing the simplest mathematical model that is believed to capture all the detail necessary and sufficient to appropriately simulate or model the physical process being addressed in the problem statement. In fact, at a basic level, this first stage is simply defining and refining the problem statement itself. Once a model has been created, then strategies for solution are developed which are constrained by the limits of the mathematical description, by the assumptions made to insure computational tractability, and by the computational resource requirements as available on the particular processor architectures or distributed computing environments. Various (possibly alternative) strategies are then selected and implemented through a suitable computational language that supports the algebraic, differential and difference calculus used, and that supports the symbolic manipulation of the computational objects themselves in order to affect linkages between various canonical computational modules. Of course, this is followed by debugging, problem or theory refinement, and general exploration or sensitivity analysis of the model itself, and eventually publication of some results... Of these levels of computational activity, the most basic level is currently probably the least supported by intelligent assisting tools. Yet this most basic level of (1) finding and expressing the appropriate mathematical model representation, (2) analyzing or ensuring its capture of essential physics, and (3) transforming it to a structure amenable for applying known solution strategies, is frequently a highly time-consuming enterprise, fraught with error and redefinition. It could be radically shortened and verified through use of reliable equation-transformation operation tools.

Most scientists carry out such initial activity off-line, and bring a more or less well defined or reasonably expressed problem statement to their workstations. However, it would be most useful if an interactive, sophisticated symbolic and numerical manipulation system could be available to scientists at this early stage of research. Scientific computing requires access to the sophisticated numerical manipulation and computation systems that would support various types of problem transformations; and symbolic reasoning is excellent for management of the flow of computational components and for developing alternative computational strategies as would occur in a planning system. Both of these features should be brought to bear at the initial problem formulation stage by allowing for altering mathematical representations, by inverting various dependency relations, by carrying out sundry symbolic substitutions and reformulations through differential operations, by reordering partial differential equations according to their symmetry bases, and by maintaining semantics throughout these transformations.

It should be noted that in considering problems in fluid dynamics and instability theory, I am not referring to problems in applied computational fluid dynamics. In that domain, simulations of complex flow fields are created around fixed aerodynamic structures in order to observe non-laminar flow fields and to define how to minimize these vortex sheets by optimally redesigning the structure. I believe that these problems are reasonably well-defined from the outset, and many years of experience has gone into creating advanced simulation and exploration tools for these researchers. Rather, here I am referring to the scientific understanding of the conditions under which various forms of turbulent transport and energy dissipation in naturally occurring fluids, such as atmospheres or planetary interiors, might grow or transform to finite amplitude secondary flow structures; or how the conditions in these fluids respond to perturbations in their flow fields so that the fluid evolves into new flow regimes. The concentration is on the fluid rather than on a structure.

The initial representation of this type of fluid dynamics problem may be a fairly broad model description at the level of the relevant equations of motion, conservation laws, constitutive equations, and boundary conditions which embed these equations into a particular problem statement. But an actual "working" problem statement arises only from successive refinements, coordinate transformations, transformations in and out of various phase space representations, substitutions of truncated power series expansions or of new parameters, and physically or mathematically justified constraints or assumptions on this initial problem statement. In a sense, the general problem is reduced to a particular instance upon which an entire intellectual fabric may hinge. For example, to study isostatic recovery flow of the Earth following deglaciation of the Pleistocene ice sheets under weakly non-Newtonian rheology, one starts with equations for conservation of momentum, of mass, and with an expression for nonlinear viscosity. After much transformation, substitution, and differential operation on these equations, one *realizes* that the essential question to be addressed is to clarify the actual role of coupling of harmonic disturbances in nonlinear stress-dependent rheology and induced wavelength harmonics. Boundary conditions are then created for *that* problem.

The realization is an act of insight which cannot be anticipated at the outset of the problem definition. It arises because of the insight gained from understanding the constraints against solution methodologies embodied in the original problem statement, the assumptions, and problem reformulation strategies. It is a kind of insight not eagerly allocated to "assisting" systems by scientists. In particular, it is a different kind of insight than that gained from detailed numerical simulation and experimentation on the "whole" model, a process frequently allocated to high speed, vector processor architectures. It is also a different form of insight from that which arises under analysis of phase portraits of dynamical systems. Phase portraits are not currently tailored to expose the detailed physical processes responsible for transitions between bifurcated regions of the phase space. Rather, they identify variations in dynamical systems behavior as gleaned from identification of initial conditions of trajectories in the phase space, or from analysis of the evolution of eigenvalues in the complex plane as particular bifurcations parameters are varied with respect to characteristic flow parameters. However, the symmetries that arise from such analysis are the same that occur in the original differential equations, and so there should be a way of mapping between these kinds of representations to achieve physical process insight.

So, why is this paper entitled "math metaphors"? Consider a language. It has a grammar by which we understand the deeper linguistic structure. At the surface, the words are used to define and individuate concepts, and the structure allows these concepts to be interrelated. Once we have learned the grammar, and at some level the linguistic structure, we study the literature. The literature is a transformation of ideas through metaphor; understanding in the language requires metaphor because this is how the unfamiliar become familiar, how new connections and relations are established. We use the language to reformulate the language.

Mathematics is also a language with a surface grammar and a deep grammatical structure. We spend many years learning the surface grammar, which is basically manipulation of symbols for identities -- everything through differential and integral calculus. The surface grammar is used to manipulate symbols which define and identify substitution possibilities wherein an equation says "the result of carrying out the calculation on the left side of the *equals* sign is the same as the result of carrying out the one on the right side." Once we get to ordinary and partial differential equations, to higher order and to nonlinear equations, or to variational calculus, we are at a new level of use in the language. There are no longer any fixed rules about what counts as a solution: a solution is any function that can be found to satisfy the equation, given the particular problem conditions. The bulk of scientific computation is this calculation by algebraic substitution of values for variables, and the substitution of calculation process for equivalent calculation process. But in science theory formation or in problem statement formulation, *prior* to these substitutions of calculations for calculations, is the metaphorical transformation of equation and model representations, operating at the level of the structure of the language, and with its attendant insight. Our theory and insight is enhanced by the metaphors we create through this analytic transformation of the problem statement. This act is not part of 'solution methodology' but rather transformation of problem representation and propagation of understanding. Just as a theory is a metaphor between model and reality, so is a problem refinement a metaphor between the original model and a solution. This level of theory formation is the level of the expressibility and subtlety of the language. It is this metaphorical level of expressibility in assisting tools that is advocated.

Discussion and Examples

In this section, I present several examples of the types of equation transformations that occur regularly in nonlinear fluids problems and in dynamical systems generally, thereby hopefully lending clarification to the ideas of the previous section. It is difficult to rank these operations according to which are the most useful or the most necessary for near-term intelligent automation. Rather, it is my hope that some of these techniques will seem within grasp to some of the AI research community, or these examples will stimulate a domain for research towards intelligent mathematical and scientific tools.

First, let us consider Burgers' equation, and look at two possible transformations of it that turn out to make it solvable by alternative methods. The appropriate form can well depend on the physical setting in which the equation arises in a given problem, so one form may be more "intuitive" than another. Burgers' equation is generally thought of as one form of mathematical model for turbulent flow, and it is also used in the approximate theory for weak stationary shock waves in real fluids. It has the general form of a quasi-linear PDE, $L[u] = 0$, and for λ a parameter, it has the form:

$$u_t + uu_x - \lambda u_{xx} = 0 \tag{1}$$

We can now construct what is called the Hopf transformation, in two steps. Introduce a new variable, v, and set $u = v_x$. Substitution yields the equation:

$$v_{xt} + v_x v_{xx} - \lambda v_{xxx} = 0 \tag{2}$$

and one integration by x yields:

$$v_t + (1/2)v_x^2 - \lambda v_{xx} = 0 \tag{3}$$

This equation looks worse than before, but if we then introduce a second transform of variables between v and a new variable w such that $v = -2\lambda \log(w)$, equation (3) reduces to a simple one-dimension diffusion equation

$$w_t - \lambda w_{xx} = 0 \tag{4}$$

which is solvable by known methods. Of course, a solution for w yields a solution for v and hence for u. The combined transformation:

$$u = -2\lambda\ [\log(w)]_x \tag{5}$$

is called the Hopf transformation. I presented it here in two stages because if we stop at equation (3) there is an alternative method of solution. Furthermore, perhaps the physical problem under consideration yields this form of transformed Burgers' equation, and the diffusion solution is not what is wanted. Equation (3) can also be solved by so-called "separation" methods. Here, a typical solution is sought in the form:

$$v = f[t + g(x)] = f(w) \tag{6}$$

for unknown f and g. Here, $w = t + g(x)$. Upon substitution of (6) into (3), a relation arises for f and g:

$$f'(w)[1 - \lambda g''(x)] = [g'(x)]^2[\lambda f'' - (1/2)(f')^2] \tag{7}$$

which can be separated into

$$\begin{aligned} [1 - \lambda g''(x)] / (g')^2 &= [\lambda f'' - (1/2)(f')^2] / f' \\ &= \text{constant} = c \end{aligned} \tag{8}$$

Hence, f and g must satisfy the system of equations:

$$\begin{aligned} \lambda f'' - (1/2)(f')^2 - cf' &= 0 \\ \lambda g'' + c(g')^2 &= 1 \end{aligned} \tag{9}$$

These equations are integrable by reduction of order. The successes from using transformations of the form (6) for Burgers' equation above has led to the generalization of such transforms for use in solutions of the Navier-Stokes equation, whereby the stream function is assumed to have the form

$$\psi = f[t + g(x) + h(y)] \tag{10}$$

and this then opens up another area of analysis for instability and turbulence.

This first example is fairly straight-forward, and is well known in the literature -- in fact, people are probably irritated at always seeing Burgers' equations examples. But here at least it introduces the flavor of transformation of equations tailored to specific needs. The point is that if access to suites of transformations were available in a computational system, then various experiments could be run by operating on the defining equations and discovering the symmetries that emerged. This would of course require not only the possibility of functional substitution, but also the availability of differential operation on equations as a whole so as to separate or project forms on subspaces or create, say, poloidal and toroidal component equations, and so on.

As a second example, consider some simple variable transformations on the Navier-Stokes equation. This equation represents conservation of momentum in fluids, and for incompressible fluids, it takes the form:

$$\partial u_i/\partial t + u_j\ \partial u_i/\partial x_j = -\ 1/\rho\ \partial p/\partial x + \nu\ [\partial^2 u_i/\partial x_i \partial x_j]$$

where i,j = 1,2,3, and u_i is velocity, ρ is density, p is pressure, and ν is constant kinematic viscosity. Because the fluid is incompressible, the conservation of mass is expressed by a simplified form of the continuity equation, namely, that div **u** = 0. That means that, for the two-dimensional problem (u,v;x,y), we can define a stream function that satisfies continuity, whereby now

$$u = \psi_y \quad \text{and} \quad v = -\psi_x \; ; \text{ with } \psi_{yx} - \psi_{xy} = 0$$

Thus one can see that the Navier-Stokes equations could be written in terms of the stream function ψ and the pressure gradients by substituting the above definitions, and carrying out the necessary differentiations. Normally, if one is proceeding along this path, one also then cross-differentiates the equations and subtracts to eliminate pressure, and the resulting equation is a fourth order PDE in the stream function. The partial derivatives have essentially projected the original equations onto a one family set of curves in "stream-function" space. But, instead of pursuing that path here (and because my final example carries it out in more detail), consider the transformation that arises from assuming a solution of the form:

$$u_i = -2\nu/\phi \, [\partial\phi/\partial x_i]$$

If this transformation is substituted into the original Navier-Stokes equation for u_i, the resulting equation is a linear diffusion equation in ϕ:

$$\partial\phi/\partial t = \nu[\partial^2\phi/\partial x_i\partial x_j] + \{p(t,x_1,x_2,x_3)/2\rho\phi\}\,\phi$$

This equation can now be thought of as a model for viscous flow in a pure initial-value problem where pressure is prescribed. In this case, it turns out that the velocity field must satisfy a source distribution of

$$S(t, x_1, x_2, x_3) = -2\nu[\partial \ln \phi/\partial x_i\partial x_j]$$

in order to guarantee that conservation of mass is still satisfied. If, however, S = 0, then the linear diffusion equation for ϕ above along with mass conservation, transforms into a Bernoulli equation, which classically relates flow to pressure and density. On the other hand, the nonlinear form of Bernoulli equation

$$\partial\theta/\partial t + 1/2\,[\partial\theta/\partial x_i \, \partial\theta/\partial x_j] + p/\rho = 0$$

goes back to a linear diffusion equation by using mass conservation and the transform $\theta = \ln \phi$.

Each of these manipulations are in the general class of reducible equations and are found in nonlinear PDE texts; they may provide guidance to scientists who are working on finding a reasonable representation for their particular problem. Such transforms and others similar would be valuable if they were available in "working" knowledge of a computationally assisting system.

Well, so much for these kinds of examples...where's all the *insight* that is supposed to arise from these transformations? Where's the ***metaphor***? To see that, we need to consider an application of these types of transformations to real problems. That is what I outline now in this final example. It is also the example to be presented in more detail at the meeting, so I will basically outline the structure and evolution of the analysis here, and leave out the more cumbersome math details.

Suppose the general problem is one of understanding the nonlinear viscosity distribution in the Earth's interior. There are several sources of data that can constrain such analysis, namely, earthquake-seismic, laboratory data on phase transitions in mantle-like rocks, gravity anomalies over large regions of the Earth, historical records on sealevel change, earthquake free-oscillation data, and changes in length of day due to tidal de-spinning of the Earth-Moon system, to name a few. It may turn out that most of this data can be supported by more simple layered linear viscosity; but for now suppose one has reason to hypothesize nonlinear viscosity. Then here is an example strategy with transformations.

The problem to be considered is the flow of the mantle of the Earth in response to the unloading (melting) of the Pleistocene ice sheets about 7K to 10K years ago. We want to determine the viscosity profile in the mantle $\mu(x,y)$ based on this flow **v**(x,y) of the mantle in response to the unloading stresses. Bold terms are vector quantities. The basic equation of motion for rebound flow in this medium is the variable viscosity form of the Navier-Stokes equation, representing conservation of momentum. In vector form this equation is:

$$\rho\, D\mathbf{v}/Dt = \rho\mathbf{g} - \nabla p + [\nabla\cdot(2\mu\nabla)]\mathbf{v} + \nabla \times (\mu\nabla \times \mathbf{v})$$

Conservation of mass is simply div **v** = 0, as before. The inertial terms in the convective derivative D**v**/Dt can be ignored in this problem because they are small compared to the viscous terms and restoring stresses. It is assumed that the flow is confined to the (x,y) plane, with y positive vertically upward from the non-deformed surface. The next usual operation is to introduce a term for the vorticity as curl **v** into the equations of motion, which then become:

$$\nabla(p + \Phi) = -\mu\nabla \times \xi + 2(\nabla\mu\cdot\nabla)\mathbf{v} + (\nabla\mu) \times \xi$$

$$\text{with} \quad \xi = \nabla \times \mathbf{v}$$

Here the gravity force is written as the gradient of a potential Φ. This equation can now be operated on by taking the curl of the whole equation (ie, ∇ x :) which eliminates the potential terms and projects the vector equation onto the (x,y) plane. This operation also serves to eliminate several of the terms in the expanded form of the differential vector operator relations. The vorticity vector itself points in the transverse plane, and its components lie entirely in (x,y). After carrying out all the operations and imposing mass conservation, the two-dimensional form of the (now) single equation of motion can be written explicitly in terms of u, v, and μ, with partial differentiation in x, y:

$$\mu(v_{xxx} - u_{xxy} + v_{xyy} - u_{yyy})$$
$$+ 2[\mu_x(v_{xx} - u_{xy}) + \mu_y(v_{xy} - u_{yy})$$
$$+ 2\mu_{xy}(v_y - u_x) + (\mu_{xx} - \mu_{yy})(v_x + u_y) = 0$$

The horizontal and vertical velocity components can again be represented in terms of a Stokes stream function $\psi(x,y)$

$$u = \psi_y \quad \text{and} \quad v = -\psi_x$$

which becomes the single dependent variable describing the flow. Substitution yields:

$$\mu(\psi_{xxxx} + 2\psi_{xxyy} + \psi_{yyyy})$$
$$+ 2[\mu_x(\psi_{xxx} + \psi_{xyy}) + \mu_y(\psi_{xxy} + \psi_{yyy})$$
$$+ 4\mu_{xy}\psi_{xy} + (\mu_{xx} - \mu_{yy})(\psi_{xx} - \psi_{yy}) = 0$$

Solution of this fourth-order, viscous-dominant equation of motion is sought in terms of $\psi(x,y)$. Integrations of ψ would then give u and v, and if an explicit relation is made for the viscosity in terms of the flow strain-rates, then this viscosity profile can be found as well. Conversely, a viscosity form can be assumed in order to start the analysis, and iterations can converge to a self-consistent system.

The problem is that the viscosity $\mu(x,y)$ is now a complicated function of the stress field or strain-rate field in the medium; hence it is also a function of $\psi(x,y)$. The equation of motion is thus highly nonlinear in $\psi(x,y)$, and exact admissible solutions are not known. One cannot assume a simple modal solution for ψ, such as a superposition of Fourier components, because in the nonlinear problem, as the deformed surface rebounds, a new stress field is induced by which given disturbance harmonics will couple and induce other harmonics. In addition, the change in strain rates during recovery will alter the viscosity profile sensed by the rebounding nonlinear fluid. That is, μ must be considered as the functional $\mu[\psi(x,y)]$. Hence, the form of a general solution to this equation of motion must be derived which is appropriate for describing the rebounding flow in such a non-Newtonian medium. Transformations (math metaphors) become necessary, because we hope to preserve physical understanding at the same time. Once a general solution $\psi(x,y)$ is found, it can be used in conjunction with various boundary conditions to develop an equation which describes the time-change (relaxation) of the deformed surface. This rate can be compared with projections from data for verification of the model.

In order to derive the general solution $\psi(x,y)$, it is necessary to impose physically reasonable assumptions on the nature of the viscosity variation, and to indicate the extent to which flow in the medium is coupled to this viscosity variation. Ideally, these assumptions should also yield mathematical tractability! I have selected a viscosity variation which can be described as weakly spatially coupled (the viscosity at one position is dependent on the viscosity of material nearby), and I have also had to assume that the stream function behaves smoothly over a narrow bandwidth about some prescribed wavelength even though the overall variation across the spectrum may be significant. These assumptions are converted to mathematical constraints on the form of the solution $\psi(x,y)$ and on the form of the transformation analysis during reduction of the equations. It turns out that this approach provides both significant physical insight into the nonlinear rheology problem as well as mathematically tractable analysis.

An acceptable method to advance beyond statement of our fourth-order equation is to Fourier Transform it, solve the resulting equation in the (k,h) transform domain for Ψ (k,h), then inverse transform this solution back to yield an analytic form for $\psi(x,y)$. This analytic form of $\psi(x,y)$ can then be differentiated appropriately, now with some understanding of the role of coupling of harmonics, and an actual relaxation equation can be developed for the rate of change of the deformed surface under specified initial displacement or stress conditions. By using our $\psi(x,y)$, and combining the expression for vanishing normal stress at the deformed free surface with a kinematic surface condition that ties the vertical velocity of that surface to the rebounding motion there, a partial differential equation is derived which describes the time evolution and rebound of the initially specified depressed land. Solution of this equation is the ultimate goal; it can be carried out numerically using finite-difference or multigrid techniques.

All work prior to this equation can be considered symbolic manipulation and exploration in theory formation and problem statement reformulation. In this summary, I have also simplified the presentation in that the analysis in the Fourier Transform domain turns out to be rather involved. The convolutions integrals that are solved in (k,h) are of course the various products in (x,y), such as $\mu_x\psi_{xyy}$, and solution of these integrals is what requires the stringent assumption on the form of nearest neighbor "awareness" of the viscosity functions. In several instances, truncated series expansions are needed, and these are substituted (more metaphor). At one point, an interesting first-order PDE arises to be solved for the transformed stream function $\Psi(k,h)$:

$$A(k,h)\ \partial\Psi(k,h)/\partial k \ +\ B(k,h)\ \partial\Psi(k,h)/\partial h$$

$$+\ C(k,h)\ \Psi(k,h) \ =\ 0$$

This equation is then solved along characteristic paths in (k,h) space by a transformation of variables. The subsidiary equation

$$dh/dk \ = B(k,h)/A(k,h)$$

$$= \text{function}(k,h,k',h')$$

defines the characteristic paths in (k,h) along which the solution must exist, and this yields a constraint on the relation between the two wavenumbers k and h (representing the transform from x and y). The primed k and h are not derivatives, but rather represent the width of the pulse for μ in the convolution integrals in the k and h directions. This constraint dictates the form of the final solution, but it also yields insight into the nature of the coupling of the harmonics from the relaxing deformation. For a suitable transformation of variables, the first-order equation above becomes:

$$A(\zeta,\theta)\ \partial\Psi(\zeta,\theta)/\partial z \ +\ C(\zeta,\theta)\ \Psi(\zeta,\theta) \ =\ 0$$

In this problem, the appropriate transformation of variables turns out to be:

$$\theta(k,h) = hk^{-b/a} \quad \text{and} \quad \zeta(k,h) = k$$

where b and a are also functions of the pulse width. This transformation leads to a solution of the first-order equation in (ζ,θ) space, and inverse transforming this yields a solution for Ψ (k,h). Finally, the Ψ (k,h) solution is inverse Fourier Transformed to yield the desired solution for our original stream function ψ (x,y). Plus, the nonlinearity of the viscosity is completely incorporated in this solution due to the convolution integrals.

This $\psi(x,y)$ can now be analytically differentiated, and finally an equation can be developed for the relaxation of the surface. It is this final equation which becomes the particular problem to be solved in this physical scenario. All the rest is preparation for that.

Summary

In this paper, I have attempted to show the variety of symbolic manipulation of equations that can occur during the initial problem statement formulation stage in a theoretical applied math problem. Frequently, scientists bring fully formed problem statements to their workstation to seek numerical solution or symbolically guided variation of parameters of a well-formed problem. However, in many of those cases, a tremendous amount of off-line analysis has been accomplished ahead of runtime, and this work I have referred to as problem statement formulation: starting from general equations of motion and transforming and reducing the equations to a solvable representation. This enterprise is in dire need of intelligent mathematical manipulation tools by which the scientist can explore various transformation possibilities and see what physical constraints are intimately tied to each kind of transformation or assumption. This theory formation stage of theoretical work requires the capability of substitution of variables, substitution of truncated series representations for variables, changes in independent variables so as to reformulate equations in alternative spaces, carrying out integrations such as Fourier Transforms so that analytic results can be viewed and manipulated, inverse transforming back retaining original meaning, and re-writing equations according to various symmetry operations or from differential vector operations. In an ideal case, a user might be able to start with conservation laws for mass, momentum, and energy, and write them as balance equations in "english" and later replace words with mathematical terms representing the processes. That would truly be metaphorical! In all of this operation, it is necessary to retain a background knowledge whereby vector symbols retain meaning or body forces really can be considered as gradients of potentials, and so on. In addition to these intelligent data structures, planning systems could be exploited to manage the progress of the calculations, while retaining the experience of alternative strategies. Understanding would then propagate through transformation.

It is my hope that these systems can come under development -- I intend to continue to work in this direction myself.