Going with the Flow: a Lagrangian approach to self-similar dynamics and its consequences

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Abstract

We present a systematic computational approach to the study of self-similar dynamics. Through the use of what can be thought of as a “dynamic pinning condition” self-similarity is factored out, and a transformed, non-local evolution equation is obtained. The approach, which is capable of treating both first and second kind self-similar solutions, yields as a byproduct the self-similarity exponents of the original dynamics. We illustrate the procedure through the porous medium equation, showing how both the Barenblatt (first kind) and the Graveleau (second kind) self-similar solutions naturally arise in this framework. We also discuss certain implications of the dynamics of the transformed equation; in particular we discuss the discrete-time implementation of the approach, and connections with time-stepper based methods for the “coarse” integration/bifurcation analysis of microscopic simulators.

1 Introduction

When one tries to computationally locate constant shape traveling wave solutions in an equation that supports them, the standard procedure is to go to a traveling frame, so as to change the time-dependent problem into a steady state one. Since, however, the correct speed is not, in general, known a priori, two possibilities exist: either we will see no steady states (having guessed the wrong speed), or we will see infinitely many (if we were
fortunate in guessing the correct speed). The simple solution to writing fixed point algorithms for this problem is to realize that one is allowed to pick one out of the one-parameter infinity of steady state solutions of the PDE in the traveling frame. One-parameter here corresponds to traveling (translational invariance, a continuous symmetry group) in one spatial dimension; the concept generalizes directly to traveling in more than one spatial dimensions. Computationally one augments the system by writing an additional (possibly nonlocal) condition, called a “pinning condition” [5]. We then have enough equations to solve for the one solution and the correct traveling speed simultaneously.

Rowley and Marsden [10] introduced recently a template-based technique for “factoring out” translational invariance; their work was motivated by the so-called Karhunen-Loeve expansion in the case of PDEs with traveling wave solutions. This was done by choosing a (more or less arbitrary) function, the template, and using it to systematically pick out one out of the one-parameter infinity of elements of the group orbit in a manner that will be explained below. We have recently implemented a discrete time version of this template-based approach to perform what we call “effective” bifurcation analysis of evolution equations in complicated media [11].

An important contribution of the work of Rowley and Marsden is that through the template method they allow the pinning to be done in a dynamic way. This means that we do not just implement some computational contraction mapping, and then converge on its fixed point, which is the solution traveling with constant speed and constant shape. Through the template we actually have a way to “factor out” the translational invariance in continuous time, and thus get an equation in an appropriate frame at all times. This is quite interesting since, often, what we want to find is not just the final solution, but we also want a view – “unobstructed” by the symmetry group – of the physical dynamics of the approach to the traveling wave. It is of course, in principle, possible to first find the traveling solution by some independent means (e.g. analytically) and then factor it out from the dynamics. The template approach allows us to do the “factoring out” of the group orbit naturally and continuously in time, without a priori knowledge of either the traveling solution or its speed. Moreover, as a simple byproduct it yields at the end the solution and the correct speed.

In this paper we extend the template approach to another continuous symmetry group: self-similarity. We take advantage of the fact that using a template to factor out self-similarity, we actually obtain a dynamic evolution equation. This equation not only gives the self-similar solutions, but it actually gives a view of the dynamics of approach to the self-similar solution
with the self-similarity conveniently factored out.

The remainder of the paper is organized as follows: in the following section we show how to derive the transformed evolution equation for the scaled variable. We then illustrate the procedure through the computation of two well-known solutions (the Barenblatt solution, a self-similar solution of the first kind, and the Graveleau solution, a self-similar solution of the second kind) through the dynamics of the transformed equation. We conclude by a discussion of what we perceive as the implications of the approach, including alternative (to integration) computational approaches to the location of self-similar solutions. We also discuss briefly the discrete-time implementation of the approach on the original (as opposed to the transformed) equation. This has possibly important implications because of the recently proposed “coarse” integration/bifurcation analysis techniques for analyzing microscopic (e.g. Molecular Dynamics (MD) or Monte Carlo (MC)) timesteppers. It is conceivable that the computer-assisted analysis of self-similarity proposed here can be carried out even in cases where coarse, macroscopic equations describing the evolution of moments of molecular distributions conceptually exist but are not available in closed form.

We also note that what we propose here shares many elements with the approaches described, for example, in page 326 of the book of Goldenfeld [8], and in Chapter 6 of [14], including references to the work of the authors of the book, as well as Papanicolaou, Zakharov and their groups. We are currently exploring the similarities and differences of our work with that literature (see also [4]).

Because of the long ties, over the years, of two of the authors with the University of Minnesota, and because this work came to fruition in an office at U of M., we will call the transformed dynamics developed here the “MN-dynamics”.

2 Self-similar solutions

Self-similar solutions play an important role in the development of the theory of nonlinear evolutions equations. In addition to providing exact and sometimes even explicit solutions they often describe the asymptotic behavior at large times, or the asymptotic form of solutions in the neighborhood of some important change in behavior such as focusing or blow-up at some finite critical time. Often a self-similar solution to an autonomous evolution
equation in the variables \((x_1, x_2, ..., x_n, t)\) is a function of the form
\[
|t - t^*|^{\beta} F\left(\frac{x_1}{|t - t^*|^{\alpha_1}}, ..., \frac{x_n}{|t - t^*|^{\alpha_n}}\right),
\]
(1)
where the similarity exponents \(\alpha_1, ..., \alpha_n, \beta\) and the function \(F\) must be determined from the equation together with appropriate boundary and initial conditions. Here \(t^*\) is either the known initial time in which case we consider \(t > t^*\), or the unknown critical time so that we consider \(t < t^*\). In view of the time translation invariance we can always take \(t^* = 0\). In some problems the exponents can be obtained \(a priori\) from scaling arguments and conservation laws. This is referred to as \textit{self-similarity of the first kind}. However, it is often the case that the exponents cannot be gotten \(a priori\) and are usually obtained by solving what amounts to a nonlinear eigenvalue problem for the function \(F\). This is the case of \textit{self-similarity of the second kind}. A cogent account of the theory of self-similar solutions with many illuminating examples can be found in Barenblatt’s book [3].

In the next section we will derive the MN-dynamics equations for the construction of self-similar solutions. In section 4 we illustrate the method by applying it to the computation of the Barenblatt solution (first kind self-similarity) and the Graveleau solution (second kind self-similarity) of the porous medium equation (pme)
\[
\frac{\partial u}{\partial t} = \Delta(u^m)
\]
where \(m > 1\) is a constant. For properties of the porous medium equation see [4].

3 MN-Dynamics

Consider the partial differential equation
\[
u_t = D_x(u),
\]
(2)
where the generally nonlinear operator \(D\) acts on the variable \(x\). We restrict ourselves to operators for which there exist two constants \(a\) and \(b\) such that for all positive \(A\) and \(B\)
\[
D_x \left( B f \left( \frac{x}{A} \right) \right) = A^a B^b D_y \left( f \left( y \right) \right), \text{ where } y = \frac{x}{A}.
\]
(3)
For these operators the PDE may have a one-parameter family of self-similar solutions
\[ u(x,t) = s^\beta U \left( \frac{x}{C s^\alpha} \right), \tag{4} \]
where \( C > 0 \) is the parameter, \( s = |t - t^*| \), and \( U \) satisfies the ODE
\[ \sigma C^{-\alpha} (\beta U - \alpha y U_y) = D_y (U) \text{ in the variable } y = \frac{x}{C s^\alpha} \tag{5} \]
with \( \sigma = sgn(t - t^*) \). The exponents \( \alpha \) and \( \beta \) satisfy the scaling condition
\[ \beta - 1 = a\alpha + b\beta. \tag{6} \]

We now present an alternative method of computing similarity solutions, which factors out the similarity exponent \( \alpha \). We start with the general scaling
\[ u(x,t) = B(s) w \left( \frac{x}{A(s)}, \tau(s) \right), \tag{7} \]
where \( A, B, \) and \( \tau \) are unknown functions. Using Eq. (3) we obtain the PDE for \( w \)
\[ \sigma \left( \frac{B_s B}{B} w - \frac{A_s}{A} y w_y + \tau_s w_{\tau} \right) = A^a B^{b-1} D_y (w) \tag{8} \]
Given an appropriate template function \( T(y) \) we want to adjust \( A(s) \) so that \( w \) satisfies the orthogonality condition
\[ \int_{-\infty}^{+\infty} w(y, \tau) T(y) dy = 0. \tag{9} \]
Multiplying Eq. (8) by \( T(y) \) and integrating we obtain
\[ \frac{A_s}{A} = -\sigma A^a B^{b-1} I(\tau), \tag{10} \]
where
\[ I(\tau) = \frac{\int_{-\infty}^{+\infty} D_y (w(y, \tau)) T(y) dy}{\int_{-\infty}^{+\infty} y w_y (y, \tau) T(y) dy}. \tag{11} \]
To determine \( B \) we need an additional pinning condition. For numerical convenience we impose the local condition \( w(p, \tau) = 1 \) at some fixed point \( x = p \). For example, \( p \) may be a symmetry point where \( w_y (p, \tau) = 0 \) for all \( \tau \). Evaluating Eq. (8) at \( y = p \) and substituting from Eq. (11) we obtain
\[ \frac{B_s}{B} = \sigma A^a B^{b-1} \left( D_y (w(p, \tau)) - p w_y (p, \tau) I(\tau) \right). \tag{12} \]
Substituting Eqs. (10) and (12) in Eq. (8) we obtain
\[ w_\tau + I(\tau) (yw_y - wpw_y(p, \tau)) + wD_y(w(p, \tau)) = D_y(w) \] (13)
provided that
\[ \tau_s(s) = \sigma A^a(s)B^{b-1}(s). \] (14)

In view of Eq. (14) we can rewrite \( A \) and \( B \) as functions of \( \tau \) instead of \( s \). Let \( \tilde{A}(\tau) = A(s(\tau)) \) and \( \tilde{B}(\tau) = B(s(\tau)) \). Then it follows from Eqs. (10), (12), and (14) that
\[ \frac{\tilde{A}_\tau}{\tilde{A}} = -I(\tau) \quad \text{and} \quad \frac{\tilde{B}_\tau}{\tilde{B}} = D_y(w(p, \tau)) - pw_y(p, \tau)I(\tau). \] (15)
Moreover, the physical time \( s = |t - t^*| \) is given as a function of \( \tau \) by
\[ \frac{ds}{d\tau} = \sigma \tilde{A}^{-a}(\tau)\tilde{B}^{1-b}(\tau). \] (16)

Starting from a suitable initial condition \( w(y, 0) \), we integrate Eq. (13) for \( \tau \to \infty \). If \( w(y, \tau) \) converges to a steady state \( W(y) \), there is a similarity solution to Eq. (2). In particular, \( W \) satisfies
\[ k (yw_y - pW_y(W)) + WD_y(W(p)) = D_y(W), \] (17)
where
\[ k = \lim_{\tau \to \infty} I(\tau) \] (18)
as well as Eq. (3). Comparing coefficients in Eqs. (3) and (17) we find that
\[ \frac{\alpha}{\beta} = \frac{-k}{D_yW(p) - kpW_y(p)}. \] (19)
Thus the similarity exponents \( \alpha \) and \( \beta \) are determined by the linear system consisting of Eqs. (6) and (19).

In problems where there is a finite critical time \( t^* \) we are interested in \( t < t^* \) so that \( \sigma = -1 \) and \( s = t^* - t \). We integrate Eqs. (13) and (16) to obtain
\[ t^* = t(\tau = 0) + \lim_{\tau \to \infty} \int_0^\tau \tilde{A}^{-a}(\eta)\tilde{B}^{1-b}(\eta)d\eta. \] (20)
A remarkable property of this method is that it is able to capture both self-similar solutions of the first and second kind, as we show in the next section.

We note that the new PDE Eq. (13) can also be obtained by repeatedly evolving Eq. (2) an infinitesimal time interval \( dt \), and then rescaling the \( x \) and \( u \) variables such that they satisfy \( u(L, t) = 1 \) and Eq. (1).
4 Examples

Here we give two examples of numerical integration of Eq. (13) to obtain self-similar solutions to the porous medium equation with \(m=2\).

The 1D Barenblatt solution is the self-similar solution of the first kind to the porous medium equation whose initial datum is a Dirac mass at the origin. This solution is known explicitly \([1]\) and

\[\alpha = -\beta = 1/3.\]

The operator in this case is \(D_x(u) = (u^2)_{xx}\) and the scaling condition Eq. (13) reduces to \(\beta = 2\alpha - 1\). We discretized the equation with centered finite differences. The time integration is carried out with an explicit Euler scheme on a domain \([0,3]\) discretized with 600 points. From the linear stability analysis of the numerical scheme, the variable time step must satisfy \(\Delta t < 0.5/|w(y,\tau)|\) on the domain of integration. To compute the Barenblatt solution we choose the template function

\[T(y) = \begin{cases} 
1 & \text{for } |y| \leq 1 \\
-1 & \text{for } |y| > 1 
\end{cases}\]

The orthogonality condition Eq. (9) means that the dimensionless mass within \(|y| \leq 1\) equals the mass outside this interval. For the initial datum we take

\[w(y,0) = \begin{cases} 
1 & \text{for } |y| \leq 2 \\
0 & \text{for } |y| > 2 
\end{cases}\]

which satisfies the orthogonality condition. Fig. 1 shows the convergence of the numerical solution to the steady state. The numerical value of the similarity exponent given by Eq. (19) is \(\alpha = 0.333371\) for \(\tau = 10\).

The Graveleau solutions to the porous medium equation form a 1-parameter family of axi-symmetric focusing solutions which are self-similar of the second kind \([2]\). To construct them by integrating the MN-dynamic equation we write the equation in \((r,t)\) coordinates. For axi-symmetric diffusion the operator is \(D_r(u) = (u^2)_{rr} + (u^2)_r/r\) and the scaling condition is again \(\beta = 2\alpha - 1\). We approximate the solution that has an infinite support with a numerical solution in a finite interval \([0,10]\), discretized with 2000 gridpoints. We use the boundary conditions \(w(0,\tau) = 0, w_y(L,\tau) = 0\), and in Eq. (13) we set \(L = 10\).

The template function is chosen to be

\[T(y) = \begin{cases} 
-1 & \text{for } 0 \leq |y| \leq 7 \\
1 & \text{for } 7 < |y| \leq 10 
\end{cases}\]
and the initial datum is
\[
w(y,0) = \begin{cases} 
0 & \text{for } 0 \leq |y| \leq 4 \\
1 & \text{for } 4 < |y| \leq 10 
\end{cases}
\]
which is orthogonal to \(T(y)\) on the integration domain. We show the evolution of \(w\) in Fig. 2. As \(\tau \to \infty\) the solution tends to a steady state. In this case the corresponding physical time tends to a finite value \(t^*\) which is the time at which the solution to the original initial value problem first becomes positive in the neighborhood of the origin. \(t^*\) is called the focusing time. To determine the similarity exponent we use Eqs. (8) and (19). For 2 space dimensions the correct value of \(\alpha = 0.856333\ldots\) and the MN-dynamics gives the approximate \(\alpha = 0.85695\). The accuracy would be improved by using more gridpoints and enlarging the domain.

5 Discussion

Locating the self-similar solutions and their exponents by integration of the MN-equation is, of course useful. It is, however, only one of the ways that we can now find these solutions. Now that the self-similar solutions have become steady states of the MN-equation, we can bring all the tools of nonlinear dynamics to bear on their study. In particular, we can find self-similar solutions not only through the fact that they may be attracting (by integration), but also through contraction mappings like Newton’s method (this would be interesting in physical problems like the Landau-Gizburg equation [15]). Indeed, we can do bifurcation / continuation / stability calculations of the closed non-local PDE and find all types of stable, unstable, bifurcating, possibly even more complicated (e.g. periodic in the transformed frame, or even more complicated, chaotic in the transformed frame) self-similar solutions. They are going to be elements of the global attractor of the MN-equation, or, in general, invariant objects for the MN-dynamics. For example, in the traveling case, a limit cycle in the transformed equation would correspond to a modulated traveling wave — so, possibly, a limit cycle of the transformed equation would correspond to a "periodically self-similar" solution for the self-similar problem. These might arise in Hopf bifurcations of the MN-equation, and might be associated with complex exponents; we are not sure at the moment what all these additional invariant objects might be, but it will be interesting to study them. We are certainly aware of cases that should correspond to steady state bifurcations in the MN-dynamics.

More importantly, however, the Jacobian of the linearization of the MN-equation at its steady states or limit cycles, should it prove to be a well
defined object, will tell us what the stability in the self-similar frame is, with the self-similarity factored out. It will help us understand asymptotic rates of approach, bifurcations of new self-similar solutions, possibly find basins of attraction of different self-similar solutions as stable manifolds of saddle-self-similar solutions. In particular, it is conceivable that in the case of Type-II self-similar solutions, continuation and the use of this linearization might facilitate the study of the post-focussing regime. There are many interesting singularities whose “other side” we would like to explore. The porous medium equation is one of them; possible examples from cosmology also come to mind.

We conclude with a few (speculative at the moment) comments.

First, when a successful transformation turns the problem of finding self-similar solutions into finding steady states, limit cycles, chaotic attractors, or in general, elements of the global attractor of the transformed dynamics, we can bring all the machinery of dynamical systems / bifurcation theory to bear on computing self-similar solutions and their transitions (bifurcations in the transformed frame). In particular, techniques much more powerful than simple integration (e.g. contraction mappings like the Newton method, continuation, and multiparameter bifurcation theory) can be brought to bear on the transformed problem.

Second, in everything we have done so far, we first transform the equation, and then work with the transformed equation. In effect, one has to write a new code to analyze the old problem. The original reason we were attracted to the template approach to factoring out translational invariance was that we were interested in using it in what in general we term ”time-stepper” based methods for numerical bifurcation theory. It is possible to implement the template procedure not only in continuous time, but also in discrete time: one runs the “original” dynamics for some time and then “pulls back” the result (as opposed to constantly pulling it back as in [4]). We have implemented this discrete time, time-stepper based bifurcation approach in [11] for the traveling case; in the same spirit, the discrete-time version of the approach can be used on the original equation in the self-similar case (as opposed to writing down the transformed MN-equation).

This opens the way for another interesting possibility. Over the last few years, we have developed methods for what we call “coarse bifurcation analysis” of microscopic time-steppers [12, 13]. In these, we create a map (using microscopic dynamics, such as Monte Carlo, or Lattice Boltzmann) from an initial condition in the space of a few moments of a distribution to a final condition (after some time) in the same truncated moments space of the distribution. The procedure involves “lifting” the macroscopic initial
condition to one or more microscopic ones conditioned on the few governing moments, running the microscopic code, and then averaging (restricting) back to governing moments space. There is a number of interesting issues about how long to run the microscopic simulator, and how to do good variance reduction, but we will not discuss this here.

Based now on the coarse-time stepper implementation, suppose that we have microscopic simulations (simulations at one level of description), and we suspect that some coarser description (moments) of the microscopic dynamics will have self-similar behavior. Then, using the coarse time-stepper and the discrete-time version of the above procedure, it is possible, given a set of reasonable assumptions discussed in some detail in [11] to find certain elements of the self-similar dynamics (e.g. steady states, invariant sets, bifurcations) of what the “coarse-MN-equation” would have been, without having to explicitly construct (approximate) this coarse-MN equation. Indeed, this approach gives rise to alternative, mathematics-motivated ensembles for performing the microscopic simulations (with an eye towards the analysis of coarse dynamics) [9]. Recent advances in multiscale computations (projective and telescopic projective integrators [6, 7], as well as what we provisionally call “patch dynamics”) may assist in doing these calculations efficiently, in smaller space and time scales than the full computational domain. These developments in multiscale computations are rather general, and not designed in particular with the coarse MN-dynamics in mind.

We believe that the general approach outlined in this paper opens new computational possibilities in the study of self-similar problems and their dependence on parameters. Problems ranging from interfacial fluid dynamics to shock waves, and from cell aggregation to cosmology and materials science may become more accessible to computer-assisted analysis, whether through closed macroscopic equations, or through the “coarse” analysis of alternative, more microscopic descriptions.

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Figure 1: Evolution of $w(y, \tau)$ for the porous medium equation. The initial rectangular profile evolves towards the steady state, keeping the scalar product with the template (dashed line) equal to zero.
Figure 2: Evolution of $w(y, \tau)$ for a convergent flow in the 2D porous medium equation. The initial rectangular profile evolves towards the steady state, which describes the selfsimilar solution before the focusing time.