Some thoughts on similarity, the POD, and finite boundaries*

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1 Introduction

This paper will take several seemingly disconnected ideas and show how they might be related. In keeping with the spirit of the Monte Verita Colloquium, I have chosen to talk about the way in which I believe the world might work in the hope that it will stimulate my own thinking and that of others. Let me begin with the physical problem which has troubled me for the two past decades: *When does a laboratory experiment or computer simulation truly represent an acceptable approximation to a flow of infinite extent?*

One can, of course, quite reasonably ask: *Who cares?* Or equally: *Why should we care?* Both questions would presumably be followed by the observation that all real flows have finite boundaries. But the simple fact is that with the exception of a few confined flows (like channel and pipe flows), almost every bit of knowledge we have about the behavior of turbulence solutions to the Navier-Stokes equations *from the equations themselves* comes from flows in which there are no boundaries. Examples include the homogeneous flows of such interest to modellers, as well as the familiar jet, wake and plume flows which are very close to flows which occur naturally. These solutions, with their simple scaling laws and similarity solutions, can be of immense value in both validating and understanding experiments,

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numerical simulations and models. And the point of this paper, departures from similarity help us understand when boundaries matter. Without this understanding, we might build models and theories for turbulence based on phenomena which have nothing to do with the dynamics of the flow, but instead are imposed by us and the domain we have chosen — and, in fact, we may have done so already. The consequences for engineering applications are of enormous importance since we seldom have the luxury of modelling (in lab or computer) a flow of realistic extent.

So when do finite boundaries matter? Now with experiments one might think the answer is obvious, but it seldom is. I first confronted this problem in 1979 when I realized that accepted measured profiles did not satisfy even the simplest momentum conservation requirements for a jet in a quiescent environment. In George (1990a) I documented four of the failures of me and my students to properly understand the subtle effects of finite boundaries — the round buoyant plume, our own round jet, grid turbulence through a contraction and free shear layers in a co-flowing stream. All of the experiments described deviated from the expected similarity results in subtle, but important, ways because of the unsuspected influence of boundaries. Since writing that article I have encountered a host of other flows where the finite boundary limits of the flow have made their presence felt, some of which I shall discuss below.

How does one *prove* the finite boundaries are important? The usual approach for the more difficult engineering problems, either computationally or experimentally, is to pretend the boundary conditions are not too important since the limitations of memory or space may leave little alternative. Sometimes an attempt is made to double the box size or move out the experimental boundaries, but more often not. Numerical studies may seek an experiment to "validate" the computation, and it is usually possible to find an experiment which does so. One surprising thing about the afore-mentioned jet measurements was that most of the experiments agreed with each other, but almost all of them were carried out in the same size room with even the same size jet. So agreement with experiment, in and of itself, should not be too satisfying. In fact, the whole point of the George (1990a) paper was that an experiment may be assumed valid *ONLY* when the data satisfy the governing equations and boundary conditions which are *ASSUMED* to apply. If they do not, then either the measurements are wrong, or the flow is not the flow it is believed to be.

The problem is a little more obscure for the the DNS and many theoretical types: Their results *always* satisfy the governing equations and imposed boundary conditions since they obtained solutions by solving them. And they have avoided the problems of the experimentalist by simply *defining* their world to be periodic (*cf* Frisch 1995, Doering and Gibbon 1996). Now while this may self-consistent, there is no assurance that these periodic results bear any resemblence to the non-periodic world around us. So how do they decide whether these results mimic reality? They can, of course, compare to experiments which are themselves done in finite boxes. Even so, the results are not always comforting. For example, I was shocked to learn some years ago that the DNS isotropic turbulence simulators usually throw away all the data prior to the peak in the derivative skewness since the rapid rise is believed to be part of the starting transient. Now if this is true, then all of the wind tunnel experiments (with a single exception) are invalid, since in all of the classic experiments the skewness continues to rise down the tunnel. In fact, if one looks at the eddy turn-over times and calculates an equivalent tunnel length for when the simulators think the data is good, this is 2 to 4 times the longest tunnels in the world. Now interestingly, the main reason experimenters don't build longer tunnels is because they believe the turbulence to be influenced by the walls when the integral scale grows to more than about a tenth of the tunnel width. Yet this is the ratio of integral scale to box size (or its spectral equivalent) at which many simulators *begin* their calculations.

Now let me make it clear that I am not questioning the validity of the DNS and LES results for periodic domains, only the degree to which they model turbulence in an infinite domain. Or put another way, my concern is about how much the results are determined by the non-linear dynamics as opposed to being dictated by the boundary conditions. And lest the experimentalists feel left out, I have exactly the same concern about experiments. Unfortunately, unlike the jet experiments cited earlier, none of the above examples provide indisputable proof (at least to some) that the finite domain adversely affects experiments and the simulations. At most they offer a clue. Nonetheless, our knowledge of even potential theory where the entire solution everywhere is determined by the boundaries should at least make us cautious. We have no corresponding theorems for turbulent flows, but certainly have no reason to discard boundaries as being important.

2 The Role of Similarity Solutions

The question then remains: How does one ever prove that boundaries are not important in a particular simulation or experiment? This is where similarity solutions are the most useful, since they prescribe exactly how the flow must evolve (at least statistically) for a particular set of boundary conditions (usually homogeneous in some sense). If the flow that is being modelled in the computer or laboratory is supposed to be similar, then it is relatively easy to conclude whether or not the boundary conditions are affecting it. So the big question is whether the flow is supposed to be similar?

Of course, it is important to build the similarity theory correctly. I addressed this subject in some detail in George (1989a) where I argued that the traditional self-preservation approach to turbulence used in most texts was fundamentally wrong. I also argued for a general approach, applicable to all equations, in which each dependent variable is allowed to have its own scale. These scales, and the relations among them, are then in turn determined by asking whether the equations admit to solutions in which all relevant terms evolve together. Sometimes they do, and sometimes they do not. This is, of course, the way classical *non-turbulence* similarity theory has always been done, but somewhere along the way the turbulence community got lost. Two surprising results of doing things correctly are that most flows require more than one velocity scale *and* retain a dependence on source conditions.

In that same article (George 1989a) I tried to codify my own *beliefs* (which certainly are not unique) into two formal conjectures :

- *Conjecture I*: If the equations of motion, boundary and initial conditions admit to similarity solutions, then the flow will *always* asymptotically behave in this manner.

- *Conjecture II*: If the equations, boundary and initial conditions governing the flow do not admit to similarity solutions, the flow will adjust itself as closely as possible to a state of full similarity.

Note that Conjecture I, if ever proven, is at least one manifestation of the long-sought-after uniqueness theorem for turbulent flows. And Conjecture II is the basis for all of the local similarity theories we hold so dear (like K41, etc.).

There are numerous recent examples that are consistent with Conjecture I; *eg* George 1992 (isotropic decay), George 1990 (isotropic scalar decay), George and Gibson 1992 (homogeneous shear flow), Moser *et al* 1996 (time-dependent wake), Ewing 1995 (axisymmetric and plane jets), Chasnov 1996 (two-dimensional turbulence), Boersma *et al* 1998 (round jets), Wosnik and George 1995 (natural convection boundary layers), and George and Castillo 1997 (boundary layers). All of these are consistent with the possibility of a similarity state which retains a dependence on initial (or upstream) conditions, contrary to the conventional wisdom. The last two show that the same considerations even apply to wall-bounded flows. Most importantly, *there still are no known exceptions* which would disprove the conjectures. In fact, one could argue that if Conjecture II were false, attempts to study canonical flows by experiments and simulations would be impossible because of the finite boundaries.

Now let's be very precise here: these remain *conjectures, and not theorems* until formally proven. And they can easily be disproven by counter-example. In fact some would argue that the failure of experiments and simulations to *always* conform disproves them. But this ignores the important question raised above about the importance of boundary conditions, which are crucial to the very existence of a similarity solution. Since for similarity theory they generally must be imposed at infinity, there can be no experiments or simulations which exactly satisfy the essential requirement to test the conjecture, *except possibly over a limited domain and/or for a limited time.* In fact I argue that the only place one could expect an experiment or simulation to provide a reasonable test of similarity theory is when the scales of the motion of importance are much smaller than the distance to the boundaries.[1] When the scales are growing in time or with streamwise distance, this means the solution is limited in its domain of applicability. OR put another way, the experiment ceases to be a valid test of the theory.

For example, in George (1992) I was able to show that a single length scale similarity theory was able to account for most of the observations in long wind tunnels (including about eight decades for spectral data), but it was not able to account for the DNS simulation results beyond what was generally believed (by the DNS community at least) to be the initial transient. Most troubling was that in the DNS results, the velocity deriva-

[1] Curiously, for grid and homogeneous shear flow turbulence this does not seem to have been pointed out before George 1992.

tive peaked whereas the similarity theory demanded that $SR_\lambda =$ *constant for fixed initial conditions*. For the wind tunnel experiments, almost all the data satisfied the similarity constraint, and the constant increased with *source* Reynolds number.. (Note that R_λ decreases during decay and the derivative skewness *increases*, contrary to the popular view that it decreases, at least for finite grid Reynolds numbers and *fixed initial conditions*) Subsequently, Huang and Leonard (1994) found that by introducing another length scale, they could account for the peak in the DNS results. The question they left unanswered is: Where does the other length scale come from[2]? A possible answer is: from the tunnel walls or the limits imposed by the computational box (or equivalently the lowest wavenumber allowed). If so then all of the departures from the simple similarity solution can be attributed to the effect of the finite boundaries.

Consider as a second example the time-dependent wake of Moser *et al* 1997 (see also Ewing 1995). The data were computed in a large DNS simulation and quickly settled into a similar state, both single point *and two-point* statistical properties. The similarity state was *not* the *self-preserving* state of classical theory where all statistical quantities are characterized by single length and velocity scales (*cf* Tennekes and Lumley 1972, Chapter 4). Instead it was the more general similarity solution of the averaged equations obtained by following the methodology of George 1989a, the most important difference being that the Reynolds shear stress scaled as $\Delta U d\delta/dt$ instead of $(\Delta U)^2$. (Note that these are the counter-parts of $U_\infty \Delta U d\delta/dx$ and $(\Delta U)^2$ for the more familiar spatially developing wake.) The most striking feature, however, was the normalized dissipation which rapidly achieved a near constant value, but then started to increase, slowly at first, then ever more rapidly. Coincident with the slow rise of the dissipation was the beginning of the breakdown of the similarity spectral scaling for the very largest wavenumbers. Prior to this breakdown, visualizations of the flow showed no discernable large scale structure, but subsequent to the breakdown of similarity the flow began to show large scale roller eddies which were clearly visible. As time evolved and the shear layer grew, the number of eddies continued to decrease until only two such eddies were present in the computational box.

Now which of these flow states was the transient and which was the asymptotic flow? Obviously the rolls were the asymptotic flow for the box in which the computation was performed. But if the purpose of the

[2]This question was first posed to me in this form by D. Ewing.

computation was to study turbulence in the absence of artificial boundary conditions, then I would argue (as did the authors) that the near similarity intermediate state was the best approximation to boundary free flow. Thus, here similarity theory is being used to bound the validity of the "experiment", and hence the boundary-independent part of the flow. Interestingly, this work was carried out using spectral techniques and periodic boundary conditions for two of the three directions, just like many other simulations on which we base much of our new understanding.

3 The POD and Galerkin Expansions

Some insight into the role of boundary conditions can be obtained using the POD (Proper Orthogonal Decomposition). These techniques are currently in vogue to generate appropriate bases for dynamical systems models of turbulence (*v* Holmes *et al* 1996), but they have been used for more than 30 years to investigate coherent structures in turbulence (*eg* Lumley 1967, George 1989b, Moin and Moser 1989). The problem was originally posed for turbulence by Lumley in the following manner: Suppose we have a random velocity field, $u_i(\cdot)$ where "$\cdot$" represents x_i, t or some subset of them. We seek to find a deterministic vector, say $\phi_i(\cdot)$ which has the maximum projection on u_i in a mean square sense; *ie* $\phi_i(\cdot)$ is chosen so that $< |u_i(\cdot)\phi_i(\cdot)|^2 >$ is maximized. The appropriate choice of $\phi_i(\cdot)$ can be shown by the calculus of variations to be given by

$$\int_{region} R_{ij}(\cdot, \cdot')\phi_j(\cdot')d(\cdot') = \lambda\phi_i(\cdot) \tag{1}$$

This is an integral equation for $\phi_i(\cdot)$ in which the kernel is given by the two-point correlation function, $R_{ij} =< u_i(\cdot)u_j(\cdot') >$. In general, equation 1 does not have a single solution but many, and their character depends on both the kernel *and* the region over which the integral is taken.

3.1 Fields of Finite Extent

The most familiar application of the POD is to flows in which the region is of finite extent in one or more directions (or time), either naturally or because of artificially imposed boundaries. It is well-known that when the POD is applied to flows which are of finite total energy, then the classical Hilbert-Schmidt theory applies. In this case there are denumerably infinite

POD modes (or eigenfunctions), and they are orthogonal. Thus the original velocity field can be reconstructed from them as

$$u_i(\cdot) = \sum_{n=1}^{\infty} a_n \phi_i^n(\cdot) \tag{2}$$

The *random* coefficients a_n are functions of the variables not used in the integral, and must be determined by projection back onto the velocity field; *ie*

$$a_n = \int_{region} u_i(\cdot) {\phi^*}_i^n(\cdot) d(\cdot) \tag{3}$$

The eigenfunctions are ordered (meaning that the lowest order eigenvalue is bigger that the next, and so on) so the representation is optimal in the sense that the fewest number of terms is required to capture the energy.

Thus the POD has provided several insights and possibilities: First, because of the finite boundaries it has produced a *denumerably infinite* set of orthogonal functions which optimally (in a mean square sense) describe the flow. Second a finite subset of these functions can be used to produce a finite number of equations for analysis. This is accomplished by using them in a Galerkin projection of the governing equations (in our case the Navier-Stokes equations). Thus by truncating after a specified number of modes, the infinitely dimensional governing equations are reduced to a finite set (*v* Holmes *et al* 1996 for details).

3.2 Are Homogeneous Fields and Periodic Fields the Same?

Really interesting things happen to the POD if the flow is homogeneous or periodic. Note that, contrary to popular assumption (especially in the DNS and LES communities), these are *not* the same thing. The velocity field is said to be *periodic* in the variable x if $u(x) = u(x+L)$ where L is the period and the dependence on the other variables has been suppressed for now, as has the fact that the field is a vector. *Homogeniety*, on the other hand, means the statistics are independent of origin. For example, if a flow is homogeneous in a single variable, say x, then the two point correlation with separations in x reduces to $R(x, x') = \tilde{R}(r)$ where $r = x' - x$ is the separation. Note that by definition, homogeneous flows are not of finite total energy since they are of infinite extent, so the Hilbert-Schmidt theory cannot apply to them. Moreover, periodic fields are of finite total energy only if a single period is considered, since otherwise they repeat to infinity.

Now if periodicity and homogeniety are so different, why does the confusion arise? The POD provides the answer. For fields homogeneous in x, equation 1 can be shown to transform to

$$\int_{-\infty}^{\infty} \tilde{R}(r)\tilde{\phi}(x+r)dr = \tilde{\lambda}\tilde{\phi}(x) \tag{4}$$

Since the $\phi(x)$ on the right hand side is a function of x only, it can be included in the integral on the left. Since there is now no x-dependence left on the right hand side, it is immediately obvious that solution itself must eliminate the x-dependence on the left hand side. Therefore the eigenfunctions must be of exponential form. The most interesting to us are solutions of the form $\tilde{\phi(x)} \sim \exp{(ikx)}$ where k is a wavenumber and *all* values of k are possible; *ie* $-\infty < k < \infty$. The coefficients, $\hat{u}(k)$, can be shown to be given by

$$\hat{u}(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} u(x)e^{-ikx}dx \tag{5}$$

and the velocity field can be reconstructed from them by

$$u(x) = \int_{-\infty}^{\infty} \hat{u}(x)e^{ikx}dk \tag{6}$$

Thus the POD for homogeneous fields reduces to the familiar *Fourier transform* which depends on the continuous variable k, so the number of eigenfunctions is *non-denumerable.*

The situation for periodic fields is almost the same, but not quite — and that little difference is at the root of the problems being addressed in this paper. Any periodic field, even a random one, can be represented by a *Fourier series*; *ie*

$$u(x) = \sum_{n=-\infty}^{\infty} a_n e^{i2\pi nx/L} \tag{7}$$

where the a_n are random and are determined in the usual manner. Using the orthogonality, the two-point correlation function can be written as

$$R(x,x') = \sum_{n=-\infty}^{\infty} < |a_n|^2 > e^{i2\pi n(x'-x)/L} \tag{8}$$

Thus the two-point correlation for periodic flows, like homogeneous flows, depends only on the difference variable $r = x' - x$. Hence the eigenvalue problem of the POD reduces to exactly the form of equation 4, except now the limits of integration are $(L/2, -L/2)$. It is easy to see that the POD modes must also be harmonic functions, like those for homogeneous flows. But there is a very important difference which is obvious from the integral: for periodic flows the wavenumber must be given by $k = 2\pi n/L$ *and* n can only take integer values! Moreover, the number of POD modes is now *denumerably infinite* instead of being *non-denumerable* (*ie* continuous in k). Moreover, *the POD modes and the Fourier modes are identical.* Thus the use of *Fourier series* to represent periodic fields is indeed optimal, at least in a mean square sense.

Now the relation between a boxed homogeneous field and a periodic field can be readily determined by noting that because the energy is made finite by the box, the Hilbert-Schmidt theory again applies; hence the number of eigenfunctions becomes denumerable. If the kernel of boxed field is now *in addition assumed to be periodic*, the Fourier series representation above follows immediately. Thus the periodic fields usually assumed for calculation are dynamically equivalent to a boxed homogeneous field with the additional assumption of periodicity of the *instantaneous* fields. The assumption of periodicity has not only made the eigenfunctions denumerable, but it has forced the phase relations of all the scales, and this must also be of particular concern for the largest ones.

Such calculations of bounded fields, like their experimental counterparts, can only be representative of homogeneous fields for scales of motion much smaller than the computational box (or lowest wavenumber) and for limited times. Whether current computations are acceptable is open to debate, but the departures from similarity theory of the three-dimensional calculations would suggest not. In fact, the success of the two length scale similarity analysis of Huang and Leonard (1994) in accounting for the DNS results is probably decisive, since the additional length scale must be externally imposed, consistent with the effect of confinement. In addition, the success of the two-dimensional simulations of Chasnov (1996) in producing similarity spectra (analogous to those suggested by George 1992 for three-dimensional turbulence) provides additional support since the range of scales in the calculation is substantially larger than is possible in three-dimensions.

3.3 Inhomogeneous fields of Infinite Extent

None of the approaches above applies to flows which are inhomogeneous, but of infinite extent (like most shear flows in the streamwise direction). In fact, it has not been at all clear until recently whether the POD integral even exists in all cases. All attempts to-date to apply the POD to the flow in these inhomogeneous directions have ended up applying the Hilbert-Schmidt theory to finite regions of the flow. And as a result, the eigenfunctions and eigenvalues found are dependent on the particular domain included in the decomposition. Clearly this is because it is the finite domain itself which is making the energy finite.

Recently, however, Ewing 1995 (see also Ewing and George 1995) was able to show that if similarity solutions of the *two-point* Reynolds stress equations were possible, then the POD could be applied *in similarity coordinates* and the eigenfunctions were harmonic functions in it. By using a logarithmic coordinate transformation he was able to identify a number of flows for which two-point similarity was possible, thus for these flows the POD modes were known analytically. Most importantly, the eigenfunctions were independent of the domain, at least in principle. For the far axisymmetric jet, the appropriate modes were

$$u(\kappa, x) \sim x^{-1} \exp(-i\kappa\xi) \tag{9}$$

where

$$\xi \equiv \ln x / L_o \tag{10}$$

and L_o is prescribed by the initial conditions.[3] Thus two-point similarity and the POD have yielded an optimal set of eigenfunctions into which the flow can be decomposed. The two point correlations, $R_{ij}(x, x') = \langle u_i(x) u_j(x') \rangle$, could all be expressed in the form,

$$R_{ij}(x, x') = Q(x, x') exp[i\kappa(\xi' - \xi)] = Q(x, x') exp[i\kappa \ln x'/x] \tag{11}$$

where $Q(x, x') = U_s(x) U_s(x') d\delta/dx$ and for this flow $U_s(x) \sim 1/x$ and $d\delta(x)/dx = constant$. Note the dependence of the correlation in similarity variables on $\xi' - \xi$, an obvious counterpart to the $x' - x$ dependence of homogeneous flows.

[3] Interestingly, no length scale can be formed for a point source jet from the two parameters available, the kinematic viscosity and the rate at which momentum is added per unit mass. Hence L_o must depend on 'finite' source effects, like perhaps $(B_o^2/M_o)^{1/2}$ where B_o is the rate of mass addition per unit mass (v George 1989a).

Now these functional forms are interesting for a couple of reasons. First, because they settle the question of whether the POD can be applied to a flow of infinite extent that is not homogeneous: It can! Second, for similarity flows of infinite extent, the optimal basis functions are analytical functions, and they are harmonic functions *in the similarity variable* $\xi = \ln x/L_o$. Third, there is a continuum of eigenfunctions since all values of the reduced wavenumber, κ, are possible; *ie* $-\infty < \kappa < \infty$. This last fact is the most interesting of all since it represents the counterpart of the homogeneous analysis above. Hence the denumerable POD modes of the Hilbert- Schmidt theory for an inhomogeneous finite energy flow have given way to the non-denumerable modes of Ewing. Thus, once again, the POD suggests that confining a flow changes the fundamental nature of it, consistent with observation.

There is at least one more interesting aspect of the these inhomogeneous eigenfunctions. It is easy to show by expanding the logarithm of equation 11 that the limiting forms of at least these inhomogeneous eigenfunctions are ordinary Fourier modes. From its Taylor expansion about $x = x'$, $\ln x'/x = (x' - x)/x + \cdots$. It follows for small values of $(x' - x)/x$ that $R_{ij} \sim \exp\left[ik(x' - x)\right]$ where k is the ordinary, but local, wavenumber defined by $k = \kappa x$. Thus the usual *assumptions* of *local* homogeniety and the use of spectral analysis for the small scale motions are justified, at least in this case. Whether this is a general property of the POD is still very much the subject of debate (*cf* Holmes *et al* 1996).

4 Other Possible Implications

In 1995 at a Stanford/Ames CTR 'tea' I asked, "Is there a need for a *SUPER-grid-scale* model?" My basic hypothesis was that the finite boundaries of experiments and computational domains prohibit a necessary flux of energy to scales larger that the size of the domain. I argued that the energy which should have left "the box" for larger scales, shows up at the largest scale available (or lowest wavenumber) and saturates it. Worse, since it ultimately must be transferred by non-linear interactions (possibly non-local) to the dissipative scales, it causes a hyper-dissipation.

The phenomenon of energy accumulation in the lowest wavenumber defining the boundary of the system is well-known in two-dimensional turbulence and is refered to as Bose condensation (Hossain *et al* 1983). Smith and Yakhot 1984 were even able to show that it was responsible for the emergence of coherent structures in two-dimensional turbulence. While an inverse energy cascade is a necessary consequence of the unique nature of two-dimensional turbulence, a continuing flux of energy to *larger* scales is also a necessary feature of any three-dimensional developing turbulent flow as well. Therefore it is not a big intellectual leap to suggest that similar effects might be important in all flows constained by boundaries. Certainly all of the phenomenon suggested above have been observed in three-dimensional flow, as described earlier, and the non-local spectral energy transfer as well (*v* Yeung *et al).* So at least an inferential case has been made that the finite box is responsible.

If the above hypothesis is correct, then it is possible that the problem imposed by the finite boundaries might be tractable, since models could conceivably be constructed to let the large scale energy leave. If so, this could have important practical implications for the engineering turbulence models. At least one test of such a super-grid scale model would be whether similarity can be maintained longer and farther than without it.

There are other possible implications for the future. First the proof of Conjecture I may follow directly from a requirement for a boundary-independent POD representation of an inhomogeneous, unbounded flow. Thus the POD may itself provide the required variational principle (George 1990), or at least be a consequence of whatever is (say a miminum entropy requirement). Second, the differences between the generalized Fourier modes of the unbounded (but inhomogeneous) similarity flows and the POD modes from the Hilbert-Schmidt theory for bounded flows may offer clues about how boundary limits affect the flow. This may lead to a proof of Conjecture II. Third, these same differences may provide general specific criteria for evaluating *when* the finite domains of experiments and simulations are too small to capture the essential dynamics of the flow.

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