Phase transition approach to detecting singularities of PDEs

By P. Stinis†

1. Motivation and objectives

The problem of how to construct mesh refinement methods and how to approach more efficiently possible singularities of partial differential equations has attracted considerable attention (see e.g. Almgren *et al.* (1998); Berger & Kohn (1988); Berger & Colella (1989); Budd *et al.* (1996); Ceniceros & Hou (2001); Landman *et al.* (1988)). At the same time, the problem of constructing dimensionally reduced models for large systems of ordinary differential equations (including the case of partial differential equations after discretization or series expansion of the solution) has also received considerable attention (e.g., see the review papers of Givon *et al.* (2004); Chorin & Stinis (2005)). The construction of an accurate reduced model has advantages beyond the obvious one of predicting the correct behavior for a reduced set of variables.

We present here an algorithm that is based on dimensional reduction and which can be used to perform mesh refinement and investigate possibly singular solutions of partial differential equations. The algorithm is inspired by constructions used in statistical mechanics to evaluate the properties of a system near a critical point (Goldenfeld (1992); Binney *et al.* (1992)). A critical point is a value for the controlling parameter of a system at which the behavior of the system changes abruptly). The idea underlying the computation of the properties at criticality is that while the form of the reduced system equations is important, one can extract even more information by looking at how the form of the reduced system is related to the form of the original (full dimensional) system (Weinberg (1983); Wilson (1983)). We extend this idea to the study of (possibly) singular solutions of partial differential equations by treating time as the controlling parameter and the instant of occurrence of a singularity as a critical value for the parameter, i.e., a critical point.

Our approach has two objectives: i) it provides a way of accurately monitoring the progress of a simulation toward under-resolution, thus providing as a by-product with the time of occurrence of the possible singularity; ii) it allows the formulation of a mesh refinement scheme which is able to reach the time of interesting dynamics of the equation much more efficiently compared to an algorithm that simply starts with the maximum available resolution.

The mesh refinement algorithm can be used to calculate the blow-up rate as we approach the singularity. This calculation can be done in three different ways: i) the direct approach where one monitors the blowing-up quantity as it approaches the singularity and uses the data to calculate the blow-up rate; ii) the "phase transition" approach (à la Wilson) (Goldenfeld (1992)) where one treats the singularity as a fixed point of the renormalization flow equation and proceeds to compute the blow-up rate via an analysis in the vicinity of the fixed point and iii) the "scaling" approach (à la Widom-Kadanoff)

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(Binney *et al.* (1992)) where one postulates the existence of scaling laws for different quantities close to the singularity, computes the associated exponents and then uses them to estimate the blow-up rate. Our algorithm allows a unified presentation of these three approaches.

The task of investigating numerically the appearance of a singularity is subtle. Clearly, since all calculations are performed with finite resolution and a singularity involves an infinity of active scales we can only come as close to the singularity as our resolution will allow. After that point, either we stop our calculations and conclude that a singularity may be present close to the time instant we stopped or we switch, if available, to a model that drains energy at the correct rate out of the set of resolved variables. We emphasize here that, up to some time, the evolution toward a near-singular solution can be identical to the evolution toward a singular solution. If we do not have enough resolution to go beyond the time instant after which the two evolutions start deviating, we cannot claim with certainty the presence of a singularity. In other words, given adequate resolution we can eliminate the possibility of a singularity. But, it may be difficult to prove through a finite calculation that a singularity exists.

The original motivation behind the development of the algorithm was the open problem of the formation of singularities in finite time for the incompressible Euler and Navier-Stokes equations of fluid mechanics. In addition to helping with the issue of singularity formation, we hope that the algorithm can be of use in the simulation of real world flows by allowing a better assessment of the onset of underresolution.

2. The main construction

Suppose that we are interested in the possible development of singularities in the solution $v(x,t)$ of a partial differential equation (PDE)

$$v_t + H(t, x, v, v_x, ...) = 0$$

where H is a generally nonlinear, operator and $x \in D \subseteq R^d$ (the constructions extend readily to the case of systems of partial differential equations). After spatial discretization or expansion of the solution in series, the PDE transforms into a system of ordinary differential equations (ODEs). For simplicity we restrict ourselves to the case of periodic boundary conditions, so that a Fourier expansion of the solution leads to system of ODEs for the Fourier coefficients. To simulate the system for the Fourier coefficients we need to truncate at some point the Fourier expansion. Let $F \cup G$ denote the set of Fourier modes retained in the series, where we have split the Fourier modes in two sets, F and G. We call the modes in F resolved and the modes in G unresolved. One can construct, in principle, an exact reduced model for the modes in F e.g. through the Mori-Zwanzig formalism (Chorin *et al.* (2002)). We do not address here the complications of constructing a good reduced model.

The main idea behind the algorithm is that the evolution of moments of the reduced set of modes, for example L_p norms of the modes in F, should be the same whether computed from the full or the reduced system. This is a generalization to time-dependent systems of the principle used in the theory of equilibrium phase transitions to compute the critical exponents (Goldenfeld (1992)). The idea underlying the computation of the critical exponents is that while the form of the reduced system equations is important, one can extract even more information by looking at how the form of the reduced system is related to the form of the original (full dimensional) system. We extend this idea to

the study of (possibly) singular solutions of partial differential equations by treating time as the controlling parameter and the instant of occurrence of a singularity as a critical value for the parameter, i.e., a critical point. We caution the reader that even though our motivation for the present construction came from the theory of equilibrium phase transitions, we do not advocate that a singularity is a phase transition in the conventional sense. It can be thought of as a transition from a strong solution to an appropriately defined weak solution but one does not have to push the analogy further. Note that the problem we are addressing is different from the subject known as dynamic critical phenomena (see Ch. 8 in Goldenfeld (1992)). There, one is interested in the computation of time-dependent quantities as a controlling parameter, other than time, reaches its critical value. In our case, time *is* the controlling parameter and we are interested in the behavior of the solution as time reaches a critical value.

The above arguments can be more precise. The original system of equations for the modes $F \cup G$ is given by

$$\frac{du(t)}{dt} = R(t, u(t)),$$

where $u = (\{u_k\}),\ k \in F \cup G$ is the vector of Fourier coefficients of u and R is the Fourier transform of the operator H. The system should be supplemented with an initial condition $u(0) = u_0$. The vector of Fourier coefficients can be written as $u = (\hat{u}, \tilde{u})$, where $\hat{u}$ are the resolved modes (those in F) and $\tilde{u}$ the unresolved ones (those in G). Similarly, for the right hand sides (r.h.s.) we have $R(t, u) = (\hat{R}(t, u), \tilde{R}(t, u))$. Note that the r.h.s. of the resolved modes involves both resolved and unresolved modes. In anticipation of the construction of a reduced model we can rewrite the r.h.s. as $R(t, u) = R^{(0)}(t, u) = (\hat{R}^{(0)}(t, u), \tilde{R}^{(0)}(t, u))$. For each mode $u_k,\ k \in F \cup G$, we can decompose $R_k^{(0)}(t, u)$ as

$$R_k^{(0)}(t, u(t)) = \sum_{i=1}^{m} a_i^{(0)} R_{ik}^{(0)}(t, u(t)).$$

Thus, the equation for the mode $u_k,\ k \in F \cup G$ is written as

$$\frac{du_k(t)}{dt} = R_k(t, u) = R_k^{(0)}(t, u(t)) = \sum_{i=1}^{m} a_i^{(0)} R_{ik}^{(0)}(t, u(t)). \tag{2.1}$$

Note that not all the coefficients $a_i^{(0)},\ i = 1, \ldots, m$ have to be non-zero. As is standard in renormalization theory (Binney *et al.* (1992)), one augments (with zero coefficients) the r.h.s. of the equations in the full system by terms whose form is the same as the terms appearing in the RHS of the equations for the reduced model. Dimensional reduction transforms the vector $a^{(0)} = (a_1^{(0)}, \ldots, a_m^{(0)})$ to $a^{(1)} = (a_1^{(1)}, \ldots, a_m^{(1)})$. The reduced model for the mode $u'_k,\ k \in F$ is given by

$$\frac{du'_k(t)}{dt} = R_k^{(1)}(t, \hat{u}'(t)) = \sum_{i=1}^{m} a_i^{(1)} R_{ik}^{(1)}(t, \hat{u}'(t)) \tag{2.2}$$

with initial condition $u'_k(0) = u_{0k}$. We emphasize that the functions $R_{ik}^{(1)},\ i = 1, \ldots, m,\ k \in F$, have the same form as the functions $R_{ik}^{(0)},\ i = 1, \ldots, m,\ k \in F$, but they depend *only* on the reduced set of modes F. This allows one to determine the relation of the full to the reduced system by focusing on the change of the vector $a^{(0)}$ to $a^{(1)}$. Also, the vectors $a^{(0)}$ and $a^{(1)}$ do not have to be constant in time. This does not change the analysis that follows.

Define m quantities $\hat{E}_i,\ i = 1, \ldots, m$ involving only modes in F. For example, these could be L_p norms of the reduced set of modes. To proceed we require that these quantities' rates of change are the same when computed from Eqs. (2.1) and (2.2), i.e.,

$$\frac{d\hat{E}_i(\hat{u})}{dt} = \frac{d\hat{E}_i(\hat{u}')}{dt},\ i = 1, \ldots, m. \tag{2.3}$$

Note that similar conditions, albeit time-independent, lie at the heart of the renormalization group theory for equilibrium systems (Binney *et al.* (1992), p. 154). In fact, it is these conditions that allow the definition and calculation of the (renormalization) matrix whose eigenvalues are used to calculate the critical exponents. In the current (time-dependent) setting, the renormalization matrix is defined by differentiating $\frac{d\hat{E}_i(\hat{u})}{dt}$ with respect to $a^{(0)}$ and using Eq. (2.3) to obtain

$$\frac{\partial}{\partial a_j^{(0)}}\left(\frac{d\hat{E}_i(\hat{u})}{dt}\right) = \sum_{k=1}^{m} \frac{\partial}{\partial a_k^{(1)}}\left(\frac{d\hat{E}_i(\hat{u}')}{dt}\right)\frac{\partial a_k^{(1)}}{\partial a_j^{(0)}},\ i, j = 1, \ldots, m. \tag{2.4}$$

We define the renormalization matrix $M_{kj} = \frac{\partial a_k^{(1)}}{\partial a_j^{(0)}},\ k, j = 1, \ldots, m$, as well as the matrices $A_{kj} = \frac{\partial}{\partial a_j^{(0)}}\left(\frac{d\hat{E}_k(\hat{u})}{dt}\right),\ k, j = 1, \ldots, m$ and $B_{kj} = \frac{\partial}{\partial a_j^{(1)}}\left(\frac{d\hat{E}_k(\hat{u}')}{dt}\right),\ k, j = 1, \ldots, m$. Equations (2.4) can be written in matrix form as

$$A = MB. \tag{2.5}$$

The entries of A describe the contributions of the different terms appearing on the r.h.s. of the full system to the rate of change of E_i. The same is true for the entries of matrix B and the reduced model.

The eigenvalues of the matrix M contain information about the behavior of the reduced system relative to the full system. In fact, they measure whether the full and reduced systems deviate or approach. In the renormalization theory of critical phenomena, the eigenvalues of M at the critical point are used to analyze the system properties close to criticality. The analysis is based on the assumption that the eigenvalues of M change slowly near the critical point so that even if one cannot compute exactly *on* the critical point, it is possible to get an accurate estimate of the critical exponents by computations near the critical point. Then, one performs a linear stability analysis near the fixed point and computes the system properties. The situation in the case of singularities of PDEs is different. In this case, the eigenvalues of M vary *most rapidly* near the singularity, due to the full system's rapid deterioration. Thus, we are not able to use linear stability analysis near the singularity. However, we are still able to extract the relevant blow-up rates.

3. The mesh refinement algorithm

We continue our presentation with the mesh refinement algorithm. The construction in the previous section requires the exact knowledge of an accurate reduced model. This means, the knowledge of *both* the functional form of the reduced model and the associated coefficient vector $a^{(1)}$. In fact, it is possible to relax this constraint by requiring the knowledge only of the functional form of the reduced model, i.e., knowledge of the vector $\hat{R}^{(1)}$ but *not* of $a^{(1)}$. This can be considered as a time-dependent generalization of the Swendsen renormalization algorithm (e.g., Ch. 5 of Binney *et al.* (1992)), even though here we do not have a statistical framework. The Swendsen algorithm is based on the

observation that knowledge of *only* the functional form of the reduced model but not necessarily of the associated coefficient vector $a^{(1)}$ is enough for computing quantities of the reduced system. In particular, the matrix B can be calculated by using the resolved modes' values as computed from the full system.

As previously mentioned, the entries of B describe the contributions of the different terms appearing on the r.h.s. of the reduced system to the rate of change of E_i (the same for the entries of matrix A and the full model). The determinant of the matrix B measures whether there is need for the *reduced* system to transfer energy to smaller scales. The time instant when $\det B$ becomes non-zero, T_B, signals the onset of energy transfer from the modes in F to the modes in G. The determinant of the matrix A measures whether there is need for the *full* system to transfer energy to smaller scales. The time instant when $\det A$ becomes non-zero, T_A, signals the onset of under-resolution of the full system. The time interval $[T_B, T_A)$ is our window of opportunity to refine the mesh, without losing accuracy and without wasting computational resources. We will use the value of $\det B$ as a criterion to decide when it is time to refine the mesh.

Note that if there exists a singularity, the interval $\Delta T = T_A - T_B$ will shrink to zero as we increase the resolution. The converse is not necessarily true. If ΔT appears to converge to zero as we increase the resolution, does not mean that there certainly exists a singularity. Since all the calculations are finite, there is only a maximum resolution that we can afford. It may well be that an even larger, and presently unattainable, resolution could reveal that there is no singularity.

The mesh refinement algorithm is given by:

Algorithm

(*a*) Choose a value for TOL. For this value of TOL run a mesh refinement calculation, starting, say, from N_{start} modes to N_{final} modes. For example, let $N_{start} = 32$ and double at each refinement until, say $N_{final} = 256$ modes. Record the values of the quantities $\hat{E}_i,\ i = 1, \ldots, m$ when $N = N_{final}$ and $|detB| = TOL$. Let's call this simulation $S1$.

(*b*) For the same value of TOL run a calculation with $N_{start} = N_{final}$ modes (for the example $N_{start} = N_{final} = 256$). Record the values of the quantities $\hat{E}_i,\ i = 1, \ldots, m$ when $|detB| = TOL$. Let's call this simulation $S2$.

(*c*) Compare to within how many digits of accuracy the quantities $\hat{E}_i,\ i = 1, \ldots, m$ computed from $S1$ and $S2$ agree. If the agreement is to within a specified accuracy, say five digits, then choose this value of TOL. If the agreement is in fewer digits, then decrease TOL (more stringent criterion) and repeat until agreement is met.

(*d*) Use the above-decided value of TOL to perform a mesh refinement calculation with a larger magnification ratio, i.e. a larger value for the ratio N_{final}/N_{start}.

The agreement in digits of accuracy between $S1$ and $S2$ depends on the form of the terms chosen for the reduced model. Even though we do not know the coefficients of the reduced model, knowledge of the correct functional form of the terms can significantly affect the accuracy of the results. This situation is well known in the numerical study of critical exponents in equilibrium phase transitions (e.g. see Ch. 5 in Binney *et al.* (1992)).

3.1. *How to compute the coefficients of the reduced model*

When we only know the functional form of the terms appearing in the reduced model but not their coefficients it is not possible to evolve a reduced system. We present a way of actually computing the coefficients of the reduced model as needed. If the quantities

$\hat{E}_i,\ i = 1, \ldots, m$ are, e.g., L_p norms of the Fourier modes, then we can multiply Eqs.(2.2) with appropriate quantities and combine with Eqs. (2.3) to get

$$\begin{aligned}
\frac{d\hat{E}_1(\hat{u})}{dt} &= \textstyle\sum_{i=1}^{m} a_i^{(1)} \hat{U}_{i1}^{(1)}(t, \hat{u}(t)) \\
\frac{d\hat{E}_2(\hat{u})}{dt} &= \textstyle\sum_{i=1}^{m} a_i^{(1)} \hat{U}_{i2}^{(1)}(t, \hat{u}(t)) \\
\cdots \qquad & = \quad \cdots \\
\frac{d\hat{E}_m(\hat{u})}{dt} &= \textstyle\sum_{i=1}^{m} a_i^{(1)} \hat{U}_{im}^{(1)}(t, \hat{u}(t))
\end{aligned}$$

where $\hat{U}_{ij}^{(1)},\ i, j = 1, \ldots, m$ are the new r.h.s. functions. Note that the r.h.s. of the equations above does not involve primed quantities. The reason is that here the reduced quantities are computed by using the values of the resolved modes from the full system. The above system of equations is a linear system of equations for the vector of coefficients $a^{(1)}$. In fact, the matrix of the system is the transpose B^T of the matrix B. The linear system can be written as

$$B^T a^{(1)} = \mathbf{e} \tag{3.1}$$

where $\mathbf{e} = \left(\frac{d\hat{E}_1(\hat{u})}{dt}, \ldots, \frac{d\hat{E}_m(\hat{u})}{dt}\right)$. This system of equations can provide us with the time evolution of the vector $a^{(1)}$.

The determination of coefficients for the reduced model through the system Eq. (3.1) is a time-dependent version of the method of moments. We specify the coefficients of the reduced model so that the reduced model reproduces the rates of change of a finite number of moments of the solution. This construction can actually be used as an adaptive way of determining a reduced model if one has access to experimental values of the rates of change of a finite number of moments. Suppose that we are conducting a real world experiment where we can compute the values of a finite number of moments on a coarse grid only. Then we can use the system Eq. (3.1) at predetermined instants to update a model defined on the coarse grid. Results of this construction will be presented elsewhere.

4. Calculation of the blow-up rate at the singularity

In this section we show how the mesh refinement algorithm can be used to compute the blow-up rate as the solution approaches the singularity. We begin with the direct approach.

4.1. *The direct approach*

We restrict ourselves to the case of an algebraic (in time) singularity, meaning that some function of the solution diverges as $\sim |T_c - T|^{-\gamma}$, where $\gamma > 0$. Let us assume that T_c is known. One obvious way of estimating γ, is to run the mesh refinement algorithm and store the values of the blow-up quantity , say $\xi_n,\ n = 1, \ldots, N$, and the instant T_n at which each refinement took place. Then, one can plot (in log-log) the values of the blow-up quantity at the different refinement instants T_n as a function of the distance from the singularity $T_c - T_n$ and estimate the slope of the curve. That would provide us with the blow-up rate. Here we are interested in showing how the same estimate can be obtained using properties of a renormalization flow, i.e., a coarse-graining (dimensional-reduction) procedure. Before proceeding, we have to address the issue of the value of T_c which is, in general, unknown. Thus, the value of T_c has to be calculated from the

algorithm. It is simple to see that small errors in the estimation of T_c can lead to large errors in the estimation of the blow-up rate. One way of estimating T_c is the following: for different choices of T_c, plot, in log-log coordinates, the values of the blow-up quantity at the refinement instants T_n as a function of the distance from the singularity $T_c - T_n$ and pick the value of T_c for which this plot is a straight line. This can be decided by monitoring the value of the correlation coefficient for a linear regression.

We present results of the above construction for the inviscid Burgers equation with the initial condition $u(x, 0) = \sin(x)$ and periodic boundary conditions in $[0, 2\pi]$. This initial condition leads to a singularity forming at time $T_c = 1$. We need to choose a reduced model for the modes in F. We use a reduced model, known as the t-model, which follows correctly the behavior of the solution to the inviscid Burgers equation even after the formation of shocks (Bernstein (2007); Hald & Stinis (2007)). The t-model was first derived in the context of irreversible statistical mechanics (Chorin *et al.* (2002)) and was later analyzed in Bernstein (2007); Hald & Stinis (2007). It is based on the assumption of the absence of time scale separation between the resolved and unresolved modes. The t-model can be brought in the form of Eq. (2.2) with $a_1^{(1)} = 1$ and $a_2^{(1)} = 1$. In fact, as stated in Sec. 3.1 one can assume as known only the functional form of the reduced model and allow the coefficients $a_1^{(1)}$ and $a_2^{(1)}$ to vary. We can then use the construction in Section 3.1 to compute the values of $a_1^{(1)}$ and $a_2^{(1)}$ as needed to satisfy the conditions of Eq. (2.3).

Figure 1 shows the log-log plot of the maximum absolute value of the velocity gradient $\log(\max|\frac{\partial u}{\partial x}|_n)$ and of the inverse distance from the singularity time $(1-T_n)^{-1}$ as recorded at the different refinement steps T_n. The slope of the curve is $\gamma = 1 \pm 10^{-8}$. Note that the minute error in the estimate shows that the refinement algorithm keeps the calculation well-resolved even very close to the singularity. The calculations were performed using the mesh refinement algorithm of Sec. 3 with the refinement tolerance criterion $TOL = \det B$ set to 10^{-10}. We should note that for this value of TOL, the value of $\det A$ for the full system is still much smaller than the double precision roundoff threshold of 10^{-16}. For this calculation we set $N_{start} = 32$ and $N_{final} = 131072$ and the algorithm terminated at time $T = 0.996$.

4.2. *The "phase transition" approach*

As previously mentioned, we are also interested in showing how the blow-up rate estimate can be obtained using properties of a renormalization flow, i.e., a coarse-graining process. The key idea is that a series of successive refinement steps (going to smaller and smaller scales) can be seen as a coarse-graining process in reverse. Thus, one can run the mesh refinement algorithm, compute and store the coefficients of the reduced model at each refinement step and then use them to reconstruct the renormalization flow from smaller to larger scales. In this case, the smallest scale that the refinement algorithm reached is the starting scale of the renormalization flow. For the case of a time-dependent PDE the mesh refinement algorithm allows us to get closer and closer to the singularity instant T_c. Thus, the renormalization procedure will take us further and further away from T_c.

There are two ways to show how the renormalization flow can be used to compute the blow-up rate. The first, the "phase transition" approach assumes that the phase transition is a fixed point of the renormalization flow and proceeds with an analysis near the fixed point (e.g., pp. 124-127 in Binney *et al.* (1992)). However, as mentioned in the discussion after Eq. (2.5), we do not use a linear stability analysis because the eigenvalues

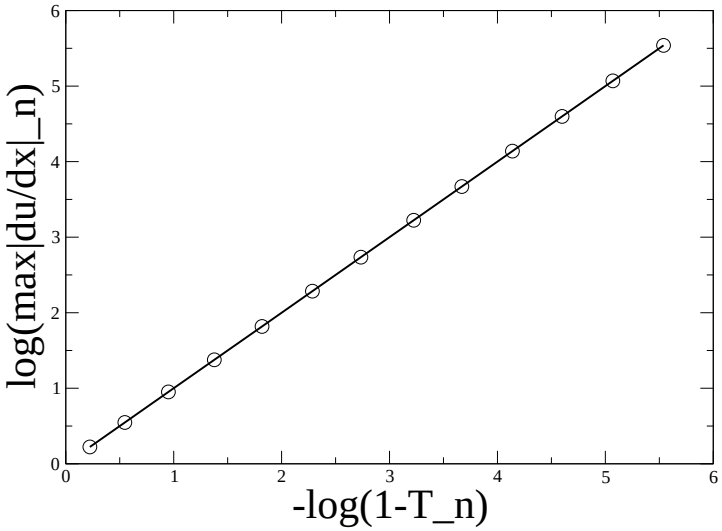

FIGURE 1. Log-log plot of the maximum absolute value of the velocity gradient $\max|\frac{\partial u}{\partial x}|_n$ and $(1-T_n)^{-1}$ for the different refinement steps (indexed by n). Algorithm ($\circ$), linear fit (—).

of M vary most rapidly near the fixed point. Instead, we deal with the full (non-linear) renormalization flow.

The second way, the "scaling" approach, is just a manipulation of different scaling laws assuming to hold asymptotically near the singularity. Of course, both lead to the same expression for the blow-up rate. We choose to present both since it elucidates further the connection between the techniques presented in this paper and those used in the theory of equilibrium phase transitions.

We start our presentation of the blow-up rate calculation with the "phase transition" approach (see e.g., Binney *et al.* (1992)). Let us suppose that near the singularity instant T_c a quantity ξ behaves as $|T_c - T|^{-\gamma}$. For the case of Burgers this would be the maximum of the velocity gradient, i.e., $\max|\frac{\partial u}{\partial x}|$. We want to find the value of γ. As previously mentioned, we assume that we have computed and stored a sequence of coefficients for the reduced model, the associated length scale, the value of the blow-up quantity and the time of occurrence of the refinement step. Then, by simply reversing the sequence indexing, we have the necessary quantities for the description of a renormalization flow which starts close to T_c and moves further away with every coarse-graining step. Since every renormalization step takes us further away from the critical point T_c, the values of the blow-up quantity become smaller with every renormalization step. Thus, if we coarse-grain the length scale at which we probe the problem by a factor of b at each step (where $b > 1$), then $\xi_{n+1} = \frac{\xi_n}{b^{\beta_2}}$, with $\beta_2 > 0$. This implies $\xi_n \sim l_n^{-\beta_2}$ and thus β_2 can be computed from the refinement algorithm data collected. The coefficient of the reduced model which monitors the deviation of the full and reduced model will increase with each renormalization step, i.e., $\alpha_{n+1} = \alpha_n b^{\beta_1}$, with $\beta_1 > 0$. This implies $\alpha_n \sim l_n^{\beta_1}$ and β_1 can also be computed from the collected data. Moreover, repeated application of the recursive relation for the coefficient α_n gives $\alpha_n = \alpha_0 (b^{\beta_1})^n$. This relation is the analog of the recursive relation derived in the theory of phase transitions by linearization

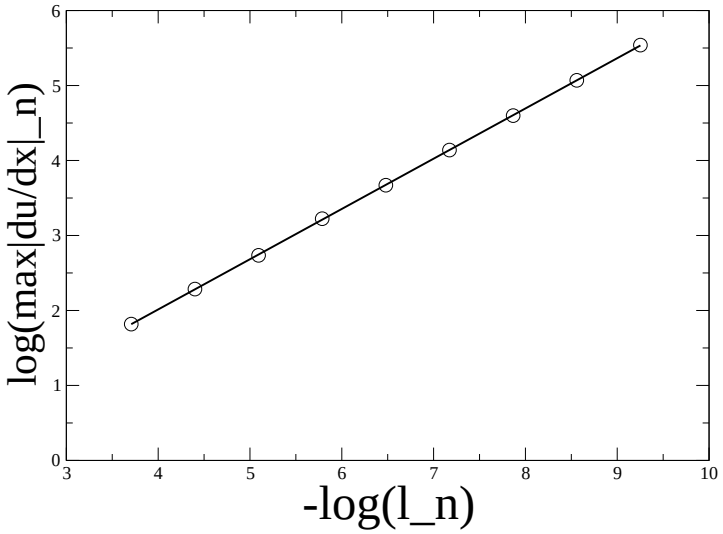

FIGURE 2. Log-log plot of the maximum absolute value of the velocity gradient $\max|\frac{\partial u}{\partial x}|_n$ and the inverse length scale of the reduced system l_n^{-1} for the different renormalization steps (indexed by n). Algorithm ($\circ$), linear fit (—).

of the renormalization flow around the critical (fixed) point. Here we did *not* resort to a linearization procedure. To proceed, we need to estimate the behavior of α_0, the starting point of the renormalization flow. In the theory of phase transitions, the behavior of the coefficient α_0 is assumed to be linear in $|T_c - T|$. However, there is no *a priori* reason for such behavior. We assume that $\alpha_0 = C_2|T_c - T|^\delta$, where δ can also be computed from the collected data.

Let us summarize what we have obtained so far. As we renormalize, the blow-up quantity decreases and the reduced model coefficient that monitors the deviation of the full and reduced model increases. Following the phase transition approach we thus assume that if we take enough renormalization steps, we then have

$$\frac{\xi}{C_1(b^{\beta_2})^n} = u \ \text{ and } \ C_2|T_c - T|^\delta (b^{\beta_1})^n = v,$$

where u, v are quantities of the same order and C_1, C_2 are constants that depend on the initial conditions. We can eliminate n in the above two relations and get

$$\xi \sim |T_c - T|^{-\gamma}, \text{ with } \gamma = \frac{\delta\beta_2}{\beta_1}.$$

Thus, we have expressed the blow-up rate exponent γ as a function of scaling exponents that are associated with properties of the renormalization flow.

Before concluding this approach, one more comment is in order. As previously stated, the "phase transition" approach treats the singularity as a fixed point of the renormalization flow. To do that, one has to construct a differential equation for the evolution of the coefficient α with respect to l. Note that by the way we have defined it, α is dimensionless. The equation for its evolution with changes in l is given by $l\frac{\partial\alpha}{\partial l} = \beta(\alpha)$

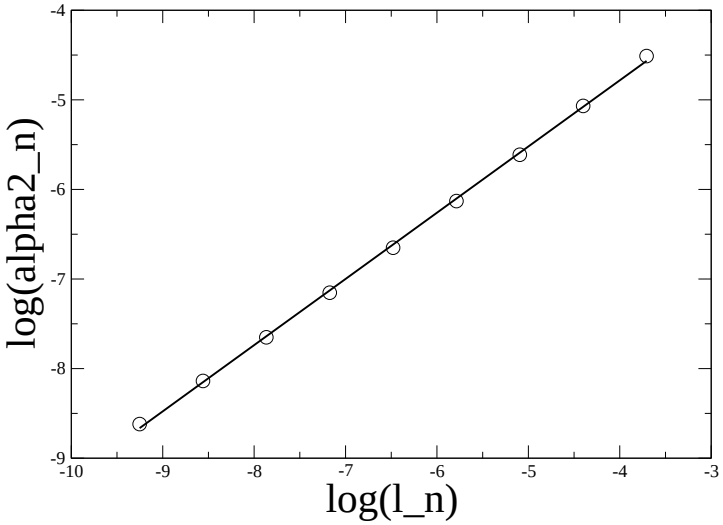

FIGURE 3. Log-log plot of the coefficient $a_2^{(n)}$ of the t-model and the length scale of the reduced system l_n for the different renormalization steps (indexed by n). Algorithm ($\circ$), linear fit (—).

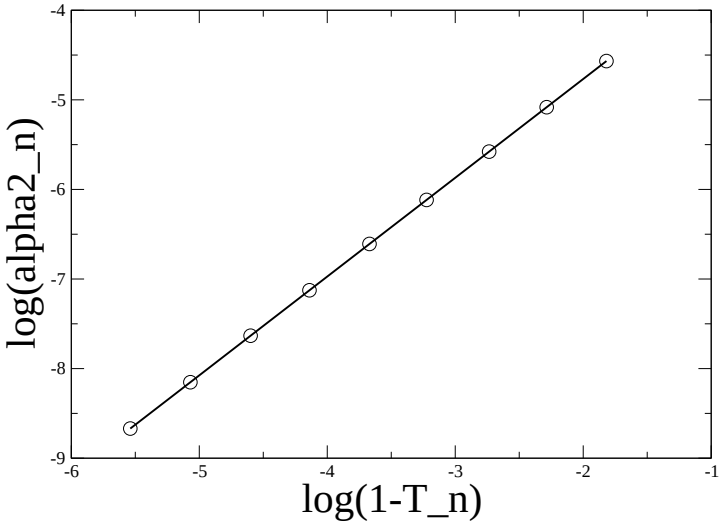

FIGURE 4. Log-log plot of the coefficient $a_2^{(n)}$ of the t-model and $1 - T_n$ for the different renormalization steps (indexed by n). Algorithm ($\circ$), linear fit (—).

(Binney *et al.* (1992)). The r.h.s. of the equation is called the beta function and its zeros determine the fixed points of the renormalization flow. Since $\alpha = Cl^{\beta_1}$, for some constant C, we have $l\frac{\partial \alpha}{\partial l} = C\beta_1 l^{\beta_1}$. So, the beta function is $\beta(\alpha) = C\beta_1 l^{\beta_1} = \beta_1 \alpha$. The only fixed point of the beta function is $\alpha = 0$. If $\beta_1 > 0$, then $\alpha = 0$ corresponds to $l = 0$, i.e., the

zero scale. But this is exactly the active scale reached at the instant that the singularity occurs. Therefore, the singularity is indeed a fixed point of the renormalization flow as long as $\beta_1 > 0$. Moreover, if $\beta_1 > 0$, this fixed point is unstable, so that if we start close to it, the renormalization flow will take us further away. This is indeed the case for the Burgers equation, as is shown numerically in the next section.

4.3. *The "scaling" approach*

The "scaling" approach is based on direct combination of the different scaling laws associated with the renormalization flow. Indeed, let $\xi \sim |T_c - T|^{-\gamma'}$, where γ' is the blow-up rate exponent to be estimated. If we assume that near T_c we have $\xi \sim l^{-\beta_2}$, $\alpha \sim l^{\beta_1}$ and $\alpha \sim |T_c - T|^{\delta}$, we can use the renormalization flow to estimate β_1, β_2 and δ. Then a straightforward combination of the three scaling laws leads to $\gamma' = \frac{\delta\beta_2}{\beta_1}$. So, $\gamma' = \gamma$ and as expected this approach leads to the same expression for the blow-up rate exponent as the "phase transition" approach.

Figures 2-4 show how the above construction can be used to estimate the blow-up rate γ from renormalization flow quantities. Recall that the coefficient of the reduced model that monitors the deviation of the reduced and full systems is $a_2^{(n)}$. Also, that the index n appearing in the figures is used now to count the renormalization steps which are the opposite of the refinement steps. The length scale l_n at which we probe the system for the different renormalization steps is the length scale of the reduced model. This means that if we have a full system calculation with N_n modes, then $l_n = 2\frac{2\pi}{N_n}$, since the reduced model has half the resolution of the full system.

From the data we estimate the exponents $\beta_2 = 0.670 \pm 0.001$, $\beta_1 = 0.739 \pm 0.007$, and $\delta = 1.1026 \pm 10^{-9}$. From these estimates we get $\gamma' = 1 \pm 0.01$. Thus, when we compute the blow-up rate using solely renormalization flow quantities, the estimation error is larger than when computing this rate directly. This is to be expected since we had to combine three empirically determined scaling laws, each one of which comes with its own error and also relies entirely on the adequacy of the reduced model. Nevertheless, the obtained accuracy is acceptable and moreover, it highlights the accuracy of the t-model for this equation.

Finally, since $\beta_1 = 0.739 > 0$, we conclude that the singularity is an unstable fixed point of the renormalization flow (see discussion at the end of Sec. 4.2).

5. Future work

We have presented a mesh refinement algorithm, inspired by renormalization constructions in critical phenomena, which allows the efficient location and approach of a possible singularity. The algorithm assumes knowledge of an accurate reduced model. In particular, it assumes knowledge of the functional form of the reduced model but not of the actual coefficients. We provide a way of computing the necessary coefficients on the fly as needed. On a theoretical level, the algorithm can be used to study the behavior of (near-) singular solutions. On the practical side, it can be used as a mesh refinement tool.

We have examined only the simple case of periodic boundary conditions and the mesh refinement performed was uniform. We plan to extend the constructions presented here to a real space formulation which will allow the treatment of non-periodic boundary conditions and more complicated geometries. In that case, one can divide the domain into subdomains and apply the mesh refinement algorithm individually in the different subdomains. In addition, the algorithm can be modified to perform mesh-coarsening after the computationally intensive time interval of the simulation has passed.

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