THE GEOMETRIC INTEGRATION OF SCALE INVARIANT ORDINARY AND PARTIAL DIFFERENTIAL EQUATIONS

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Abstract

This review paper examines a synthesis of adaptive mesh methods with the use of symmetry to solve ordinary and partial differential equations. It looks at the effectiveness of numerical methods in preserving geometric structures of the underlying equations such as scaling invariance, conservation laws and solution orderings. Studies are made of a series of examples including the porous medium equation and the nonlinear Schrödinger equation.

KEY WORDS: Mesh adaption, self-similar solution, scaling invariance, conservation laws, maximum principles, equidistribution.

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1 Introduction

When we wish to find a numerical approximation to the solution of a partial differential equation, a natural technique is to discretise the PDE so that local truncation errors are small, and to then solve the resulting discretisation. This procedure of course underpins much of current numerical software and when linked with an effective error control strategy can lead to accurate answers. However, it does not take into account the qualitative and global features of the partial differential equation directly (although a good scheme would always aim to reproduce these in a limit). It can be argued that the global structures can often tell us more about the partial differential equation than the local information given by the expression of the equation in terms of differentials.

The recent growth in the field of geometric integration has, in contrast, led to the development of numerical methods which systematically incorporate qualitative information into their structure. Much of this work has been in the area of ordinary differential equations, and a review of this can be found in [10]. However, less has been done with numerical methods for partial differential equations which are often perceived as rather difficult infinite dimensional limits of systems of ordinary differential equations. In actual fact, the strong structure imposed by a partial differential equation on the ordinary differential equations which may (for example) arise from a semi-discretisation of it, can if anything make the application of geometric ideas rather simpler.

Obviously there are many possible qualitative features that may be present in a partial differential equation and we will not attempt to list them all here. However, a possible partial listing is as follows.

1. *Symmetries* Many partial differential equations have geometric symmetries (reflexions in space or reversibility in time), translational symmetries (in space and time) and deeper symmetries that link spatial and temporal effects (such as scaling and inversion symmetries). These symmetries are fundamental to the underlying physics that the equation represents and are often more important than the equation itself.

2. *Asymptotics* Does the partial differential equation evolve in time so that its dynamics in some sense simplifies? For example does it ultimately evolve on a low dimensional attractor, is its dynamics determined by an inertial manifold inside an absorbing ball? Do complex structures starting from arbitrary initial data simplify into more regular patterns? Does the partial differential equation form singularities in a finite time?

3. *Invariants* Are quantities such as energy, momentum or potential vorticity conserved either globally or along trajectories? Do the equations have a symplectic structure? Is phase space volume conserved?

4. *Orderings* Does the partial differential equation preserve orderings? For example if $u_0(x)$ and $v_0(x)$ are two sets of initial data leading to solutions $u(x,t)$ and $v(x,t)$ then does $u_0(x) < v_0(x)$ for all x imply that $u(x,t) < v(x,t)$? A closely related concept, important in numerical weather forcasting [14], is whether the convexity (in space) of a function $u(x,t)$ (for example pressure), is conserved during the evolution.

It is worth emphasising that these global properties are not independent and are often closely linked. For example, if the partial differential equation is derived from a variational principle linked to a Lagrangian function, then, from Noether's theorem [32], each continuous symmetry of the Lagrangian leads directly to a conservation law for the underlying equation. Symmetry when coupled with orderings frequently leads to an understanding of the asymptotic structure of the equation. Also, singularities in the equation often have more local symmetry than the general solution of the equation.

We are thus naturally drawn to ask the question of how much of this qualitative structure can be preserved by a numerical method. Of course some of these questions have been considered for some time, for example the energy preserving schemes introduced by Arakawa [1] and schemes for ordinary differential equations that conserve Lie point symmetries [25]. Furthermore, for some specific problems such as Hamiltonian ODEs or time-reversible systems, some excellent geometry preserving integrators have been developed which can be analysed using backward error analysis [36]. However, a general theory, applicable to a wide class of problems is still lacking. In this review we will look in more detail at some of the items above and then see how well numerical methods do when trying to reproduce some of the qualitative structures.

2 Symmetry

In this section we will very briefly review some of the ideas of symmetry which apply to partial differential equations in time and in one spatial dimension. We will mostly be concerned here with continuous symmetries. For a review of discrete symmetries (such as reflexional symmetries and symmetries described by finite groups) see the excellent book [21].

Suppose that $u(x,t)$ satisfies a partial differential equation

$$N(u, u_x, u_{xx}, u_t, u_{tt}, x, t) = 0. \tag{2.1}$$

We define a *symmetry* of this equation to be any transformation of u, x and t which leaves the underlying equation unchanged.

Such symmetries can be expressed in terms of actions on the tanjent bundle TM of the solution space, or more globally as transformations of the underlying variables (t, x, u) to $(\bar{t}, \bar{x}, \bar{u})$ of the form

$$\bar{t} = \bar{t}(t, x, u), \quad \bar{x} = \bar{x}(t, x, u), \quad \bar{u} = \bar{u}(t, x, u), \tag{2.2}$$

so that $(\bar{t}, \bar{x}, \bar{u})$ satisfies the same equation as (t, x, u).

The general theory of such transformations is very rich and can be found in [32], [18]. See also [16], [17] for a discussion of symmetries of difference equations. Given a partial differential equation, there are systematic procedures for finding the symmetries, which generally reduce to solving an over-determined set of linear equations. Much of this can be automated, and various computer algebra packages exist to do the calculations [29]. Having found the symmetries it is then possible to go on to find exact solutions of the differential equation in many cases.

Because the theory of symmetries of partial differential equations is so large, we will not attempt to summarise all of it here, but will instead mainly look at the important sub-class of symmetries which are given by *scaling transformations.*

Typically these take the form of maps

$$t \to \lambda^{\alpha_0} t, \quad x \to \lambda^{\alpha_1} x, \quad u \to \lambda^{\alpha_2} u. \tag{2.3}$$

Here λ is considered to be an arbitrary positive quantity. Very similar transformations also apply to systems of partial and ordinary differential equations and to partial differential equations in many spatial dimensions.

The book [2] gives many examples of systems of partial differential equations with such symmetries. These arise very naturally in many problems as they express the way that a differential equation changes when the units of measurement in which it is expressed also change. For example, if u is a velocity, then a scaling of time t by λ leads to a scaling of u by $1/\lambda$.

It is an observed fact [2] that scaling (power-law) relationships have wide applications in science and in engineering. Far from being an approximation of the actual behaviour of the equations, such scalings give evidence of deep properties of the phenomena they represent, which may have no intrinsic time or length scale and which have solutions that 'reproduce themselves in time and space' under rescaling. This is an example of a covariance principle in physics that *the underlying solutions of a partial differential equation representing a physical phenomenon should not have a form which depends upon the location of the observer or the units that the observer is using to measure the system.*

Indeed, far from being a special case, scaling symmetries of the form (2.3) are universal in physics. They can be found, for example, in fluid mechanics , turbulence [27], elasticity [13], the theory of detonation and combustion [42], [3], [38], quantum physics, heat diffusion, convection, filtration, gas dynamics, mathematical biology [31], and structural geology [9]. Scaling invariance is also, of course, closely tied up with the theory of fractals [19], and with the general theory of dimensional analysis and renormalisation [4], [20].

Motivated by the definition (2.3) we introduce a vector $\alpha = (\alpha_0, \alpha_1, \alpha_2, ..)$ to describe the scaling group. It is evident that for any such α the vector $\mu\alpha$ also describes the same scaling transformation. It is quite possible for the same system of partial differential equations to be invariant under several such scaling transformations. It is then easy to check that the scaling operations described by two separate vectors commute. Indeed, the set of vectors corresponding to scaling transformations which leave the partial differential equation invariant form a *commutative vector space.*

Self-similar solutions

Because of the richness in the behaviour of solutions to partial differential equations, which may have arbitrary initial conditions and complex boundary conditions, it is unlikely that the general solution of the partial differential equation will itself be invariant under the action of the symmetries that leave the equation invariant. For example, the nonlinear wave equation is invariant under translations in space and time. However, only those solutions which are travelling waves retain this property.

Solutions which are so invariant are termed *self-similar solutions*. Such solutions play an important role in applied mathematics (witness the importance of travelling wave solutions). Under certain circumstances they can be attractors [26], [40]. They also can differentiate between different types of initial data which lead to qualitatively different forms of solution behaviour. More significantly, they often describe the *intermediate asymptotics* of a problem [42], [2]. That is, the behaviour of an evolutionary system at sufficiently long times so that the effects of initial data are not important, but before times in which the effects of boundary conditions dominate the solution. A self-similar solution also satisfies a *simpler* equation than the underlying partial differential equation. Indeed they often satisfy an ordinary differential equation. This has made them popular for computation - although they are normally singular, homoclinic or heteroclinic solutions of the ordinary differential equation and thus still remain a numerical challenge.

A most significant feature of self-similar solutions is that they need not be invariant under the full group of symmetries that leave the underlying equations invariant. In particular they may only be invariant under a particular sub-group. We see this clearly with the nonlinear wave equation

$$u_{tt} = u_{xx} + f(u).$$

For a general function $f(u)$ this equation is invariant under the two individual translation group actions $t \to t + \lambda$ and $x \to x + \mu$ as well as the combined action

$$\theta : t \to t + \lambda, \quad x \to x + c\lambda.$$

The latter group leaves invariant a travelling wave solution moving at a speed c. A solution $u(x,t)$ of the nonlinear wave equation which is invariant under the action of θ must take the form $u(x,t) = v(x - ct)$ and the function $v(y)$ then satisfies the ordinary differential equation

$$c^2 v_{yy} = v_{yy} + f(v).$$

In this equation the wave speed c is an unknown (it is a nonlinear eigenvalue) and its value must be determined as part of the solution. More generally, for a partial differential equation invariant under the action of several groups, determining the group under which the self-similar solution is invariant will form part of the solution process and any numerical method for solving them should take this into account. Problems of this kind are called *self-similar solutions of the second kind* [42], [22]. Most problems are of this kind!

In certain special cases the precise group action can be determined from other considerations (such as dimensional analysis). This is of considerable advantage when computing the solution. For example if the wave speed of the travelling wave is known then the mesh can be required to move along with the solution. Such (less common) problems are called *self-similar solutions of the first kind.*

We now give three examples of partial differential equations with scaling invariance. These examples are meant to illustrate some of the range of behaviour which can occur. We consider numerical computations of each of these using invariant methods in Section 6 and will show how each such method can be derived by using geometrical methods.

Example 1. The porous medium equation

This an example of a problem which has self-similar solutions of the first kind. The porous medium equation models the flow of a liquid through a porous medium such as fractured rock, its mathematical theory is described in [40]. The porous medium equation is given by

$$u_t = (uu_x)_x. \tag{2.4}$$

This equation admits four continuous transformation groups, the two groups of translations in time and space and the two dimensional vector space of scaling symmetry groups spanned by the vectors

$$\alpha = (1, 1/2, 0) \quad \text{and} \quad \alpha = (1, 0, -1).$$

The porous medium equation admits a family of self-similar solutions of the form

$$u(x,t) = t^{\gamma} v(x/t^{\beta}) \tag{2.5}$$

for any values of β and γ which satisfy the algebraic condition

$$2\beta - \gamma = 1.$$

Without additional conditions any such solution is possible, however, if we impose the condition that $u(x,t)$ decays as $|x| \to \infty$ then a simple calculation shows that if the mass M of the solution is given by

$$M = \int u(x,t)\ dx \tag{2.6}$$

then M is constant for all t. The only self-similar solution with this property has $\gamma = -1/3$ and $\beta = 1/3$. Thus it is a self-similar solution of the first kind. Reducing the partial differential equation down to an ordinary differential equation and solving this gives a one-parameter family of compactly supported self-similar solutions of the form

$$u(x,t) = t^{-1/3}(a - x^2/t^{2/3})_+.$$

These solutions were discovered independently by Barenblatt and Pattle [2].

Example 2. The radially symmetric cubic nonlinear Schrödinger equation

The radially symmetric solutions of the cubic nonlinear Schrödinger equation satisfy the following PDE

$$iu_t + u_{xx} + \frac{d-1}{x} u_x + u|u|^2 = 0. \tag{2.7}$$

Where d is the dimension of the problem and x is the distance from the origin. This Hamiltonian partial differential equation models the modulational instability of water waves, plasma waves and it is important in nonlinear optics. In one dimension ($d = 1$) the partial differential equation is integrable by the inverse scattering transformation and has many symmetries and invariants. Numerical methods have been designed to incorporate these symmetries and they are (in a discrete sense) also integrable. Details are given in [30]. In higher dimensions (such as $d = 2$ or $d = 3$) the equation is no longer integrable and the solutions may blow up at the point $x = 0$ in a finite time T. In this case the partial differential equation has two significant symmetries. The scaling symmetry

$$(T - t) \to \lambda^2 (T - t), \quad x \to \lambda x \quad u \to u/\lambda \tag{2.8}$$

and the phase symmetry

$$u \to e^{i\varphi} u, \quad \varphi \in R. \tag{2.9}$$

Both symmetries act on the self-similar solutions which correspond to solutions that blow up in a finite time. These all take the singular form [41]

$$u(x,t) = \frac{1}{\sqrt{2a(T-t)}} e^{-i\log(T-t)/2a} Q(x/\sqrt{2a(T-t)}), \tag{2.10}$$

where $Q(y)$ satisfies a complex ODE. Here the scalar a represents the coupling between the amplitude and the phase of the solution and it is exactly analogous to the wave speed of the nonlinear wave equation. The value of a is a-priori unknown and must be determined as part of the solution. Thus this is an example of a self-similar solution of the second kind. The Hamiltonian for this problem is given by

$$H(u) = \int_0^\infty \left(|u_x|^2 - \frac{1}{2}|u|^4 \right) x^{d-1} \, dx, \tag{2.11}$$

and is a constant of the evolution. Substituting (2.10) into (2.11), we find that

$$H(u) = (T-t)^{(d-4)/4} \int_0^\infty \left(|Q_y|^2 - \frac{1}{2}|Q|^4 \right) y^{d-1} \, dy. \tag{2.12}$$

Thus $H(u)$ can only be constant (indeed bounded) if

$$\int_0^\infty \left(|Q_y|^2 - \frac{1}{2}|Q|^4 \right) y^{d-1} \, dy = 0. \tag{2.13}$$

It is this additional equation which determines implicitly the value of a. Details of this problem are given in [39]

Example 3. The Heat equation

The well known linear heat equation

$$u_t = u_{xx} \tag{2.14}$$

is invariant under six independent symmetries [32], of which two are the groups describing translations in time and space, one is the scaling of u given by $u \to \lambda u$ so that $\alpha = (0,0,1)$, and another is the scaling given by

$$x \to \lambda x, \quad t \to \lambda^2 t$$

so that $\alpha = (2,1,0)$. Obviously any linear combination of these gives an admitted symmetry, and we may consider a general self-similar solution to be of the form

$$u(x,t) = t^\gamma v((x-x_0)/t^{1/2}). \tag{2.15}$$

The value of γ is unknown a-priori and thus we again have a self-similar solution of the second kind. Interestingly the value of γ may change during the evolution. Consider a bounded domain $x \in [0,1]$ with Dirichlet boundary conditions

$$u(0) = u(1) = 0.$$

If the initial conditions for $u(x,t)$ are highly localised (for example a Dirac measure centred on x_0) then initially the effect of the boundary conditions on the function $u(x,t)$ will be exponentially small. Consequently, the solution takes the approximate form of the free space fundamental solution for which $\gamma = -1/2$ and

$$u(x,t) = \frac{A}{\sqrt{t}} e^{-(x-x_0)^2/4t}, \tag{2.16}$$

for a suitable constant A. After a period of time proportional to the minimum of x_0^2 and $(1-x_0)^2$ one or other of the boundaries begins to have an effect. Without loss of generality this boundary condition is at $x = 0$. In this case the boundary condition at $x = 1$ again has only exponentially small effect. The effect of this boundary at $x = 0$ is to change the value of γ so that now $\gamma = -1$. In this case there is a self-similar solution of the form

$$u(x,t) = \frac{Bx}{(t-t_0)^{3/2}} e^{-x^2/4(t-t_0)}. \tag{2.17}$$

Here B is a constant and t_0 is an effective initial time at which the boundary condition at $x = 0$ becomes important. For much greater times when the boundary condition at $x = 1$ also becomes significant, this solution is also not appropriate, and indeed the function $u(x,t)$ rapidly decays to zero. The above calculation is described in [2] where it is observed that the solution has two quite different self-similar forms for different ranges of t and between these two forms the solution has a non self-similar transitionary form.

Examples two and three are highly instructive from the point of view of a numerical approximation to the solutions of scale invariant problems. Given an equation with a known symmetry group it is natural to exploit this when solving it numerically. For example, with the porous medium equation, we might consider rescaling the problem into new variables $v = t^{1/3}u$ and $y = x/t^{1/3}$. The advantage of doing this is that such variables will vary slowly during the course of the evolution of u and hence error estimates based upon higher derivatives in these variables will be much smaller, and indeed may be uniformly bounded. However, the two latter examples illustrate a problem with this approach. We simply may not know in advance which variables to use, or indeed the self-similar variables may only be appropriate for part of the evolution of the solution. Consequently we must use a more general approach and consider numerical methods which themselves, rather than imposing coordinates on the method, scale in a similar way to the underlying partial differential equation. If this is achievable then many of the desirable structures of the original system will be preserved in discrete form. This approach is at the heart of the geometric method of integrating scale invariant equations and we will develop it further in the examples considered in Section 6.

3 Symmetry and the maximum principle

Before considering numerical discretisations of scale invariant problems, it is worthwhile also looking at the role played by the maximum principle as the combination of the maximum principle and scaling invariance tells us a great deal about the asymptotic behaviour of the underlying partial differential equation. Suppose that we have a partial differential equation from which may be derived a semi-group operator φ_t such that if $u(x,0)$ is some initial data then $u(x,t) = \varphi_t(u(x,0))$. Such a partial differential equation has a strong maximum principle if the ordering of solutions is preserved under the action of the semi-group [35]. Thus if $u(x,0) < v(x,0)$ for all x then $\varphi_t(u) < \varphi_t(v)$ for all x

and $t > 0$. Many parabolic partial differential equations (for example the nonlinear heat equation $u_t = u_{xx} + f(u)$) satisfy a strong maximum principle. Such maximum principles are invaluable when studying the dynamics of the equation. For example, if $v(x,t)$ is a known solution which is bounded above and which satisfies the partial differential equation and if $u(x,0) < v(x,0)$, then we have that $u(x,t)$ is also bounded above. Such an exact solution could easily be a self-similar solution. Furthermore, if v_1 and v_2 are two self similar solutions such that $v_1 \to v_2$ as $t \to \infty$ then if $v_1(x,0) < u(x,0) < v_2(x,0)$ we deduce immediately that $u \to v_2$. Here we see the regularising effect of the partial differential equation. Techniques similar to this are described in [40] to prove the L_1 global attractivity of the self-similar solution of the porous medium equation - although there are considerable additional analytic difficulties due to the existence of a nonregular interface. A numerical method which has both a strong maximum principle and discrete self-similar solutions will, similarly, give the correct global asymptotic behaviour of the underlying partial differential equation. This is precisely what we seek to achieve using a geometric integration approach.

4 Scaling and adaptivity

We have shown in Section 2 that scaling invariance plays an important role in the theory and behaviour of the solutions to a partial (and indeed ordinary) differential equation. It is desirable that a numerical method to discretise such an equation should have a similar invariance principle. Ideally such a numerical method should posses *discrete self-similar solutions* which are scale invariant and which uniformly approximate the true self-similar solutions of the partial differential equation over all times. If these are global attractors (or at least have the same local stability as the underlying PDE) then we will have a numerical method which has the correct asymptotic properties and indeed may have excellent accuracy when approximating singular solutions.

Scaling invariance of a partial or ordinary differential equation and adaptivity of the spatial and temporal meshes fit very naturally together. This is because the use of a fixed mesh in a discretisation automatically imposes an underlying spatial and temporal scale on the problem. This makes it impossible to consider scale invariant solutions. This difficulty disappears when we introduce adaptivity as now the spatial and temporal grids become part of the solution and can easily adjust to any appropriate length and time scale consistent with the underlying problem. When considering such an approach, it is natural to look at methods of *r-adaptivity* in which spatial mesh points are moved during the solution process, rather than *h-adaptivity* in which new points are added or *p-adaptivity* in which the accuracy of the solution approximation is increased in order. The reason for doing this is that then the solution approximation, spatial and temporal mesh become one (large) dynamical system which has a lot of structure, reflecting the underlying scalings of the original problem, and this structure can then be analysed by using dynamical systems methods. A very general account of the interaction between adaptivity in space on a moving mesh for problems with a wide class of symmetries is given by the work of Dorodnitsyn and his group [16], [17] etc. In this paper we will look at the specific case of scaling symmetries and will call a numerical method which inherits the underlying symmetries of the system *scale invariant*.

The advantage of using an adaptive method which is invariant under the action of a group, is that such methods should, if correctly designed, admit exact discrete self-similar solutions. If we conserve maximum principles and the stability of the underlying self-similar solution, then such numerical methods will have excellent asymptotic properties. However, the discrete self-similar solutions will not be the only solutions admitted by the numerical method and thus the effect of boundary conditions and arbitrary initial conditions may be taken into account. Thus, the synthesis of adaptivity with symmetry invariance provides a flexible, general and powerful numerical tool. We will see this by looking at several examples.

To make things more precise, in this case we consider a partial differential equation of the form

$$u_t = f(u, u_x, u_{xx}). \tag{4.1}$$

We may consider a fully discrete method for solving this which gives an approximation $U_{m,n}$ on a spatial and temporal mesh $(X_{m,n}, T_m)$ so that

$$U_{m,n} \approx u(X_{m,n}, T_m).$$

Here we consider discretisations with a fixed number N of spatial mesh points $X_{m,n}$, $n = 1, .., N$, for each time level T_m. In an adaptive scheme the values of $X_{m,n}$ and T_m are computed along with the solution $U_{m,n}$. Suppose that, in the absence of boundary conditions, the differential equation (4.1) is invariant under the action of the scaling tansformation

$$t \to \lambda^{\alpha_0} t, \quad x \to \lambda^{\alpha_1} x, \quad u \to \lambda^{\alpha_2} u. \tag{4.2}$$

Now, consider the approximation $(U_{m,n}, X_{m,n}, T_m)$ to $u(x,t)$ obtained by our method, so that $(U_{m,n}, X_{m,n}, T_m)$ is the solution of a discrete scheme. We say that the numerical method is *scale invariant* if (again in the absence of boundary conditions) the set of points

$$(\lambda^{\alpha_2} U_{m,n}, \lambda^{\alpha_1} X_{m,n}, \lambda^{\alpha_0} T_m) \tag{4.3}$$

is also a solution of the discrete system.

The condition (4.3) gives a means of defining conditions for an adaptive mesh. Observe that these are *global* conditions related to underlying scaling properties of the equation, rather than the usual *local* conditions of adaptivity in which (for example) we may choose to cluster mesh points where the local truncation error of the solution is high. The reason for this choice of condition on the mesh is that it accurately reflects the underlying geometry of the problem. For scale invariant ODEs the two approaches (global and local) can in fact be equivalent and lead to the same time steps. Details of this equivalence are given in [11].

As a feature of this geometry, consider *discrete self-similar* solutions. A self-similar solution of (4.1) satisfies

$$u(\lambda^{\alpha_1} x, \lambda^{\alpha_0} t) = \lambda^{\alpha_2} u(x,t)$$

so that

$$u(x,t) = t^{\alpha_2/\alpha_0} v(x/t^{\alpha_1/\alpha_0})$$

where the function $v(y)$ satisfies an ordinary differential equation. In comparison a discrete self-similar solution which has the same invariance must satisfy the condition

$$T_m = \lambda^{\alpha_0 m} T_1, \quad X_{m,n} = \lambda^{\alpha_1 m} Y_n, \quad U_{m,n} = \lambda^{\alpha_2 m} V_n \tag{4.4}$$

The existence of such a discrete self-similar solution follows immediately from the scaling invariance condition (4.3). The vectors V_n and Y_n then satisfy an algebraic equation. Now, it is easy to verify that the two operations of rescaling a partial differential equation and discretising the same equation *commute*, with details given in [11]. It follows that if the discretisation of the PDE is consistent with the underlying PDE then the algebraic equation satisfied by Y_n and V_n is a consistent discretisation of the ordinary differential equation satisfied by $v(y)$. Hence $V_n \approx v(Y_n)$. Observe that the error implicit in this approximation *does not depend upon the value of* m. Hence we may uniformly approximate the self-similar solution over arbitrarily long times. More details of this calculation are given in [11], [7] and in the following sections.

The process of introducing adaptivity is very closely linked with rescaling. Suppose that τ and ξ are computational variables in the sense of [23]. We can consider an adaptive mesh $(X_{m,n}, T_m)$ to be a *map* from the computational space (ξ, τ) to the underlying space (x, t) over which the PDE is defined, which is given in terms of the maps $X(\tau, \xi)$ and $T(\tau)$. If the computational space is covered by a uniform mesh of spacing $(\Delta\xi, \Delta\tau)$ then we have

$$T_m = T(m\Delta\tau) \quad \text{and} \quad X_{m,n} = X(m\Delta\tau, n\Delta\xi).$$

(A similar procedure can also be used in higher spatial dimensions [24].) The differential equation (4.1) when expressed in terms of the computational variables then becomes

$$u_\tau - u_x X_\tau = T_\tau f(u, u_x, u_{xx}), \quad \text{with} \quad u_x = u_\xi / X_\xi \quad \text{etc..} \tag{4.5}$$

which retains the same invariance to scaling as (4.1). An r-adaptive approach is then equivalent to discretising the equation (4.5) in the computational variables.

An essential part of this process is the determination of suitable functions $X(\tau, \xi)$ and $T(\tau)$. There is much arbitrariness about how this may be done, but we are guided in our choice by the scaling invariance condition (4.3). In particular, if we have a set of conditions for the mesh which lead to the solutions $T(\tau)$, $X(\tau, \xi)$, and $U(\tau, \xi)$ then these conditions should also admit a rescaled solution of the form $\lambda^{\alpha_0} T(\tau)$, $\lambda^{\alpha_1} X(\tau, \xi)$, and $\lambda^{\alpha_2} U(\tau, \xi)$.

There are various ways of obtaining such conditions. A popular choice for determing the function T is the Sundman transformation [28] in which a function $g(u)$ is introduced so that

$$\frac{dT}{d\tau} = g(u). \tag{4.6}$$

For scale invariance we require that $g(u)$ should satisfy the condition

$$g(\lambda^{\alpha_2} u) = \lambda^{\alpha_0} g(u). \tag{4.7}$$

In [11] a systematic method of calculating such functions is given for both single ordinary differential equations and systems of such equations.

Strategies for calculating the mesh function X vary in the literature. One direct method is to mimic the formula for T and to introduce a further function H such that

$$\frac{\partial X}{\partial \tau} = H(X, U). \tag{4.8}$$

This is a natural strategy for certain hyperbolic equations as it can correspond to advecting the mesh along the flow of the solution, see [37] where it is combined with a powerful multi-symplectic approach to study various problems in fluid mechanics. A similar strategy is also adopted by Dorodnitsyn and his co-workers for a general class of groups [16]. To give a scale invariant scheme we require that $H(X,U)$ satisfy

$$H(\lambda^{\alpha_1}X, \lambda^{\alpha_2}U) = \lambda^{\alpha_1}H(X,U) \tag{4.9}$$

or equivalently, on differentiating with respect to λ, the function H should satisfy the linear hyperbolic partial differential equation

$$\alpha_1 X H_X + \alpha_2 U H_U = \alpha_1 H. \tag{4.10}$$

A disadvantage of this approach it that it is rather local in form and it can freeze the location of the mesh, ie. it can fail to move mesh points into regions of interest such as developing singularities.

An alternative approach is to use the ideas of equidistribution, introduced by Dorfi and Drury [15] and developed by Russell and his co-workers [23]. In this approach we introduce a monitor function $M(x,u,u_x)$ and aim to equidistribute this function over the mesh. Examples of such functions are the local truncation error of the solution [33], the commonly used arc-length

$$M(x,u,u_x) = \sqrt{1+u_x^2}, \tag{4.11}$$

and more simply (and especially useful when we need to cluster points where the solution is large)

$$M(x,u,u_x) = u^\gamma. \tag{4.12}$$

Suppose (without much loss of generality) that the function $u(x,t)$ is defined on the interval $x \in [0,1]$ and the computational domain is $\xi \in [0,1]$ so that $X(0,t) = 0$ and $X(1,t) = 1$. In its simplest form, equidistribution takes the form [23]

$$\int_0^X M dx = \xi \int_0^1 M dx. \tag{4.13}$$

Observe that this principle is closely related to the geometric idea of conserving the function M over mesh intervals, and we can exploit this feature to help design meshes which automatically retain invariants of the evolution [7]. Differentiating (4.13) we have that X satisfies the moving mesh partial differential equation

$$(MX_\xi)_\xi = 0. \tag{4.14}$$

This problem is scale invariant if M satisfies an equation of the form

$$M(\lambda^{\alpha_1}x, \lambda^{\alpha_2}u, \lambda^{\alpha_2-\alpha_1}u_x) = \lambda^{\alpha_3}M(x,u,u_x) \tag{4.15}$$

where the value of α_3 can be very general, meaning that (4.14) can be invariant for a wide variety of different scalings.

We see significantly that the monitor function $M = u^\gamma$ satisfies this condition for any choice of α_i whereas the arc-length monitor function $\sqrt{1+u_x^2}$ only satisfies it in the very restrictive case of $\alpha_1 = \alpha_2$. Thus arc-length does not fit in well with the theory of invariant methods, although we will see in Section 6 that it can still be used for scale invariant problems. In contrast, it was shown in [11] that taking M to be relative local truncation error for a scale invariant ordinary differential equation, often automatically ensures that the equation (4.15) is satisfied. For this reason the choice of local truncation error for M may be a wise one!

In practice the equation (4.14) can lead to instabilities [23], even if a scale invariant monitor function is used [8]. Furthermore, it requires the use of a mesh which is initially equidistributed and this can be hard to achieve. To allow both for arbitrary intial meshes and to stabilise the system, a relaxed form of (4.14) is often used. One of the more common versions is the so called MMPDE6 which takes the form

$$-\varepsilon X_{t\xi\xi} = (MX_\xi)_\xi \tag{4.16}$$

where $\varepsilon > 0$ is a small relaxation parameter. This equation has been used with great success in many applications, see the review in [23] and a study of its applications to singular problems in [8].

The scale invariance of the equation MMPDE6 can be ensured by a suitable choice of M. This must now satisfy the more restrictive condition that

$$M(\lambda^{\alpha_1}x, \lambda^{\alpha_2}u, \lambda^{\alpha_2-\alpha_1}u_x) = \lambda^{-\alpha_0}M(x, u, u_x). \tag{4.17}$$

For example, if $\alpha_0 = 1, \alpha_1 = 1/2, \alpha_2 = -1$ and $M = u^\gamma$ then (4.16) is scale invariant when

$$\gamma = 1, \quad M(u) = u.$$

The distinction between the two conditions (4.15) and (4.17) is not important if a single scaling group acts on the system. However in problems, such as the linear heat equation discussed in the examples of the last section, where several groups act, the equation (4.14) is invariant under all such actions whereas (4.16) will (in general) only be invariant under the action of one scaling group.

Once a time-stepping and mesh adaption strategy has been formulated, the equations (4.5), (4.6) and one of (4.8), (4.14) and (4.16) can be solved using a suitable discretisation scheme. Here we discretise the problem in terms of the computational variables τ and ξ. In much work on adaptivity the underlying equation (4.5) is solved (using say a collocation method) to a higher degree of accuracy than the mesh equations (4.6), (4.8), (4.14) and (4.16). However, for scaling invariant problems this may be an unwise strategy. For such problems the close coupling of the solution with space and time means that a reduction in accuracy of the solution of the mesh equations may convert to a reduction in accuracy of the solution of the underlying partial differential equation. In particular we may wish to employ the numerical method to solve a partial differential equation from an arbitrary initial state which we believe converges toward a self-similar solution. In this case the methods described above will admit such a solution and if the mesh equations are solved accurately then the self-similar solution will be computed accurately with uniformly bounded errors.

We now consider putting this methodology into practice by looking at several case studies.

5 Scale invariant ordinary differential equations

Allowing a little more generality than the previous section we consider systems of ordinary differential equations of the form

$$\frac{du_i}{dt} = f_i(u_1, .., u_N), \quad i = 1, .., N, \tag{5.1}$$

for which there is an invariance of the form

$$t \to \lambda^{\alpha_0} t, \quad u_i \to \lambda^{\alpha_i} u_i. \tag{5.2}$$

Here we review some of the results in [11].

The self-similar solutions of this system (up to translations and refelxions in t) take the form

$$u_i = t^{\alpha_i/\alpha_0} v_i \tag{5.3}$$

where the constants v_i satisfy a suitable algebraic equation. To calculate a general class of solutions of (5.1) including the self-similar solutions we introduce a computational variable τ defined through the equation (4.5) so that we solve the transformed system

$$\frac{du_i}{d\tau} = g(u_1, .., u_N) f_i(u_1, .., u_N), \quad \frac{dT}{d\tau} = g(u_1, .., u_N). \tag{5.4}$$

This system is scale invariant provided that the function $g(u)$ satisfies

$$g(\lambda^{\alpha_1} u_1, .., \lambda^{\alpha_N} u_N) = \lambda^{\alpha_0} g(u_1, .., u_N). \tag{5.5}$$

Suppose now that we discretise the complete system (5.4) for the unknowns $u_1, .., u_N, T$ using a linear multi-step method (or indeed a Runge-Kutta method) with a discrete (fixed) computational time step $\Delta\tau$. Suppose further that this method has a local truncation error of $\mathcal{O}\left(\Delta\tau^{p+1}\right)$. Then, it is shown in [11] that for sufficiently small $\Delta\tau$, the resulting discrete system has discrete self-similar solutions $U_{i,n}$ taking the form

$$U_{i,n} = V_i z^{\alpha_i n}, \quad t_n = a + b z^{\alpha_0 n}, \tag{5.6}$$

for suitable constants V_i, a, b and z. Significantly, the discrete self-similar solution approximates the true self-similar solution with uniform accuracy *for all times* with a relative error that does not grow with time. We state this result as follows.

Theorem *Let $u_i(t)$ be a self-similar solution of the ordinary differential equation, then there is a discrete self-similar solution $(U_{i,n}, t_n)$ of the discrete scheme such that for all n*

$$u_i(t_n) = U_{i,n}(1 + C_{i,n} \Delta\tau^p). \tag{5.7}$$

Here $C_{i,n}$ is bounded for all n, independently of n.

Observe that this result does not depend upon the form of the self-similar solution. Thus, if this solution is developing a singularity (for example in the problem of gravitational collapse) the discrete self-similar solution continues to approximate it with uniform accuracy [11].

A proof of this result is given in [11]. We can go further with this analysis. The most interesting physical self-similar solutions are those which are attractors as they then determine the asymptotic behaviour of the solution. In [11] it is shown further that if the true self-similar solution is locally stable then so is the the discrete self-similar solution (5.6). In particular, if we introduce a small perturbation of the form

$$U_{i,n} = z^{\alpha_i n} \left[V_i + a_{i,n}\right], \quad t_n = z^{\alpha_0 n} \left[T + b_n\right],$$

then if $a_{i,n}$ and b_n are initially small, then they remain small for all n.

We illustrate the conclusions of this theorem by considering a simple example. Suppose that $u(t)$ satisfies the ordinary differential equation

$$du/dt = -u^3, \quad u(0) = u_0.$$

This is invariant under the transformation

$$t \to \lambda t, \quad u \to \lambda^{-1/2} u.$$

If we set $g(u) = 1/u^2$ in (5.4) then we have

$$du/d\tau = -u, \quad dt/d\tau = 1/u^2 \tag{5.8}$$

with $u(0) = u_0$, $t(0) = 0$. It is easy to see that the equation (5.8) is scale invariant, so that if $(u(\tau), t(\tau))$ is a solution then so is $(\lambda^{-1/2}u(\tau), \lambda t(\tau))$. Observe that we have linearised the equation for u. We now discretise (5.8) using (for ease of exposition) the trapezium rule. This gives

$$U_{n+1} - U_n = -\frac{\Delta\tau}{2}\left(U_n + U_{n+1}\right), \quad t_{n+1} - t_n = \frac{\Delta\tau}{2}\left(\frac{1}{U_n^2} + \frac{1}{U_{n+1}^2}\right). \tag{5.9}$$

with $U_0 = u_0$ and $t_0 = 0$. This scale invariant discretisation admits a discrete self-similar solution of the form

$$U_n = Vy^n, \quad t_n = a + by^{-2n} \tag{5.10}$$

where $V, y = z^{-1/2}, a$ and b are to be determined. Substituting into the first equation in (5.9) (and dividing by the constant factor of Vy^n) we have

$$y - 1 = -\frac{\Delta\tau}{2}(y+1)$$

so that

$$y = \left(1 - \frac{\Delta\tau}{2}\right) / \left(1 + \frac{\Delta\tau}{2}\right) = e^{-\Delta\tau} + \mathcal{O}(\Delta\tau^3).$$

Here we will assume that $\Delta\tau < 2$ so that $0 < y < 1$ and $u_n \to 0$ as $n \to \infty$. Similarly, from the second equation in (5.9) we have (on division by the constant factor of y^{-2n})

$$b(y^{-2} - 1) = \frac{\Delta\tau}{2} V^{-2}(y^{-2} + 1).$$

Hence, combining results gives

$$b = \frac{\Delta\tau}{2} V^{-2}\left(\frac{1+y^2}{1-y^2}\right), \quad y = \frac{1 - \Delta\tau/2}{1 + \Delta\tau/2}. \tag{5.11}$$

Applying the initial conditions also gives $V = u_0$ and $a + b = 0$. Thus

$$b = \left[\frac{1}{2} + \frac{\Delta\tau^2}{8} + \mathcal{O}(\Delta\tau^3)\right] u_0^{-2}.$$

Hence, from the identity

$$t_n = a + bz^{-2n} = a + b(u_0/U_n)^2$$

we have

$$t_n = \left[\frac{1}{2} + \frac{\Delta\tau^2}{8} + \mathcal{O}(\Delta\tau^3)\right]\left(U_n^{-2} - u_0^{-2}\right).$$

After some manipulation we then have

$$U_n = u_0\sqrt{\frac{1 + \frac{\Delta\tau^2}{4} + \mathcal{O}(\Delta\tau^3)}{2t_n u_0^2 + 1 + \frac{\Delta\tau^2}{4} + \mathcal{O}(\Delta\tau^3)}}. \tag{5.12}$$

We now compare the expression (5.12) with the exact solution which is given by

$$u(t) = u_0\sqrt{\frac{1}{2tu_0^2 + 1}}. \tag{5.13}$$

This is, in fact, a self-similar solution with respect to the translated time $s = t + u_0^{-2}/2$. Expanding the expression for U_n and rearranging, then gives (for the case $t_n > 0$)

$$U_n - u(t_n) = \frac{1}{16u_0 t_n}\Delta\tau^2 + \mathcal{O}(\Delta\tau^3).$$

Observe that this error is (i) of the correct order for the trapezium rule and (ii) the error *decays* as $t_n \to \infty$.

6 Scale Invariant Partial Differential Equations

As it is difficult to give a general theory for the convergence of numerical methods for scale invariant partial differential equations, we consider numerical methods as applied to the three examples described in Section 2. To simplify our discussions, we consider the case of semi-discretisations only. These results can then easily be extended to full discretisations by using the theory outlined in the previous section.

6.1 The porous medium equation

Some of these results can be found in the paper [7]. As described, the equation

$$u_t = (uu_x)_x = (u^2/2)_{xx},$$

has self-similar solutions of constant first integral (2.6). Both these, and the solution from general compactly supported initial data, are compactly supported and have interfaces at points s_- and s_+ which move at a finite speed. To discretise this equation we introduce an adaptive mesh $X(\xi, t)$ such that $X(0, t) = s_-$ and $X(1, t) = s_+$. To determine X we use a monitor function and a moving mesh partial differential equation. As the evolution of the porous medium equation is fairly gentle it is possible to use the mesh equation (4.13) without fear of instability in the mesh. This then allows a wide possible choice of scale invariant monitor functions of the form $M(u) = u^\gamma$. A convenient function to use is

$$M(u) = u,$$

the choice of which is strongly motivated by the conservation law

$$\int_{s_-}^{s_+} u\, dx = C.$$

Here C is a constant which we can take to equal 1 without loss of generality. Setting $M = u$ and $C = 1$ in (4.13) gives

$$\int_{s_-}^{X} u\,dx = \xi \tag{6.1}$$

so that on differentiation with respect to ξ we have

$$uX_\xi = 1 \tag{6.2}$$

as the equation for the mesh which we will discretise. Note that this is invariant under the group action $u \to \lambda^{-1/3}u, \quad X \to \lambda^{1/3}X$. Now, differentiating (6.1) with respect to t gives

$$0 = X_t u + \int_{s_-}^{X} u_t\,dx = X_t u + \int_{s_-}^{X} (uu_x)_x\,dx = u(X_t + u_x).$$

Thus, for the continuous problem we also have that X satisfies the equation

$$X_t = -u_x. \tag{6.3}$$

Substituting (6.2) and (6.3) into the rescaled equation (4.5) gives, after some manipulation, the following equation for u in the computational coordinates:

$$u(\xi,t)_t = \frac{1}{2}u^2(u^2)_{\xi\xi}. \tag{6.4}$$

The equations (6.2),(6.3) and (6.4) have a set of self-similar solutions of the form

$$\hat{u}(\xi,t) = (t+C)^{-1/3}w(\xi), \quad \hat{X}(\xi,t) = (t-C)^{1/3}Y(\xi), \tag{6.5}$$

where C is arbitrary and the functions w and Y satisfy differential equations in ξ only. Now, consider semi-discretisations of (6.2) and (6.4) so that we introduce discrete approximations $U_i(t)$ and $X_i(t)$ to the continuous functions $u(\xi,t)$ and $X(\xi,t)$ over the computational mesh

$$\xi = i/N, \quad 1 \leqslant i \leqslant (N-1)$$

with $U_0(t) = U_N(t) = 0$. A simple centred semi-discretisation of (6.4) for $1 \leqslant i \leqslant (N-1)$ is given by

$$\frac{dU_i}{dt} = \frac{N^2}{2}U_i^2\left(U_{i+1}^2 - 2U_i^2 + U_{i-1}^2\right). \tag{6.6}$$

To define the mesh X_i we discretise (6.2) to give the algebraic system

$$(X_{i+1} - X_i)(U_{i+1} + U_i) = 2/N, \quad 0 \leqslant i \leqslant (N-1). \tag{6.7}$$

We observe that this procedure has the geometric property of automatically conserving the discrete mass

$$\sum_{i=0}^{N-1}(X_{i+1} - X_i)\,(U_{i+1} + U_i)\,. \tag{6.8}$$

An additional equation is needed to close the set of equations for the unknowns X_i and we do this by insisting that (as in the true solution) the discrete centre of mass is conserved (without loss of generality at 0), so that

$$\sum_{i=0}^{N-1}(X_{i+1}^2 - X_i^2)(U_{i+1} + U_i) = 0. \tag{6.9}$$

Observe that the equation (6.6) for the solution and the equations (6.7), (6.9) for the mesh have decoupled in this system. This makes it much easier to analyse. We discuss generalisations of this principle in a forthcoming paper [12]. In particular (6.6) has two key geometrical features. *Firstly*, it is invariant under the group action

$$t \to \lambda t, \quad U_i \to \lambda^{-1/3} U_i.$$

Thus it admits a (semi) discrete self-similar solution of the form

$$\hat{U}_i(t) = (t + C)^{-1/3} W_i \tag{6.10}$$

where $W_i > 0$ satisfies an algebraic equation approximating the differential equation for $w(\xi)$. Observe that for all C we have

$$t^{1/3} \hat{U}_i \to W_i.$$

Secondly, the discretisation satisfies a maximum principle, so that if $U_i(t)$ and $V_i(t)$ are two solutions with $U_i(0) < V_i(0)$ for all i then $U_i(t) < V_i(t)$ for all i. (See [12]).

The consequences of these two results are profound. Suppose that $U_i(0) > 0$ is a general set of initial data. By choosing values of C appropriately (say $C = t_0$ and $C = t_1$) we can find values such that

$$t_0^{-1/3} W_i < U_i(0) < t_1^{-1/3} W_i, \quad 1 \leqslant i \leqslant N-1.$$

Consequently, applying the maximum principle to the self-similar solution we then have that for all t

$$(t + t_0)^{-1/3} W_i < U_i(t) < (t + t_1)^{-1/3} W_i, \quad 1 \leqslant i \leqslant N-1,$$

and hence we have the convergence result

$$t^{1/3} U_i(t) \to W_i, \tag{6.11}$$

showing that the solution U_i and hence the mesh X_i converges *globally* to the self-similar solution. Hence the numerical scheme is predicting precisely the correct asymptotic behaviour. This is because the discretisation has the same underlying geometry as the partial differential equation.

We illustrate this result by performing a computation. Since the equations for the solution and the equations for the mesh are decoupled, we may consider them separately. Firstly, the ODEs for the solution u in the computational domain are integrated usind a third order BDF method. We can then simply solve for the mesh by inverting a linear system at each time level, assuming we have symmetric initial data so that the centre of mass is at $x = 0$. Figure 6.1 shows a solution with arbitrary initial data being *squeezed* between two discrete self-similar solutions. The self-similar solutions shown here are those with C taking the values 0.9 and 2.3.

6.2 The nonlinear Schrödinger equation

We will summarise the method described in [5] for computing the radially symmetric blow-up solutions of the nonlinear Schrödinger equation (2.7) which become infinite at the

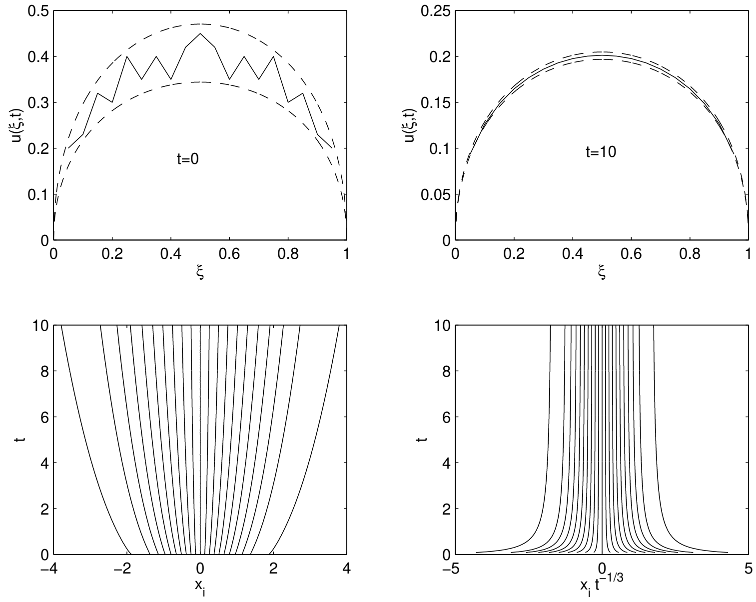

Figure 6.1: Convergence of the solution in the computational domain and invariance of the computed mesh

origin in a finite time T. Previous computations [39] have used the method of *dynamic rescaling* which is closely related to scale invariant methods, but lacks the generality of the approach we describe. The equation (2.7) is invariant under the action of the two groups (2.8), (2.9), with an unknown coupling constant a. It is immediate from the phase invariance (2.9) that the required monitor function $M(x, u, u_x)$ must be of the form

$$M(x, u, u_x) = M(x, |u|, |u_x|).$$

The mesh equation (4.14) applied to solutions which become infinite in a finite time leads to unstable meshes, and instead we use the stabilised equation (4.16). As a possible ansatz for a monitor function leading to solutions invariant under the scaling (2.8) we may use

$$M(x, |u|, |u_x|) = x^{\alpha}|u|^{\beta}|u_x|^{\gamma},$$

with the simplest scale invariant choice being

$$M = |u|^2. \tag{6.12}$$

Observe that this function is now invariant under both of the symmetries (2.8),(2.9) in the problem and hence under any combination of them. Thus the method does not need informing of the value of the coupling constant a. As an aside, the underlying partial differential equation is unitary and conserves the integral

$$\int_0^{\infty} |u|^2 x^{d-1}\, dx \tag{6.13}$$

during the evolution. Unlike the example of the porous medium equation, the monitor function (6.12) *does not* enforce this conservation law. Although this may appear to be a difficulty, in fact it is an advantage of the method. Adaptive procedures which do enforce (6.13) move points away from the developing singularity, as it is easy to show that across the developing peak of the solution, the integral of $|u|^2 x^{d-1}$ tends to zero if $d > 2$, and the integral (6.13) comes from the 'non-singular' part of the solution which does not need to be resolved with a fine mesh.

To compute the blow-up solution the rescaled equation (4.5) and the moving mesh partial differential equations (4.16) are semi-discretised by using collocation method over a large domain so that $X(0,t) = 0$ and $X(1,t) = 5$. To help with the stability of the solution the monitor function is smoothed over several adjacent mesh points. The resulting system of ordinary differential equations are then solved using DDASSL [34]. Observe that they automatically admit a self-similar solution of the form (2.10) as a special class of solutions for any value of the coupling constant a. We observe, without proof, that both the true and the (semi) discrete self-simlar solutions are stable attractors.

The resulting scheme has proved very effective at computing the singular solutions with a modest number ($N = 81$) of mesh points in the computational domain. The computations have revealed much new structure, including observations of the behaviour of multi-bump self-similar solutions when $d > 2$ [5]. We present results of a computation which evolves towards the singular blow-up self-similar solution which has a monotone profile. Figure 6.2 shows two solutions taken when $d = 3$ and the estimated value of T is $T = 0.0343013614215$. These two solutions are taken close to the blow-up time when the amplitude of $|u|$ is around 10^5 and the peak has width around 10^{-5}. Observe that the resolution of the peak is very good, indicating that the mesh points are adapting correctly.

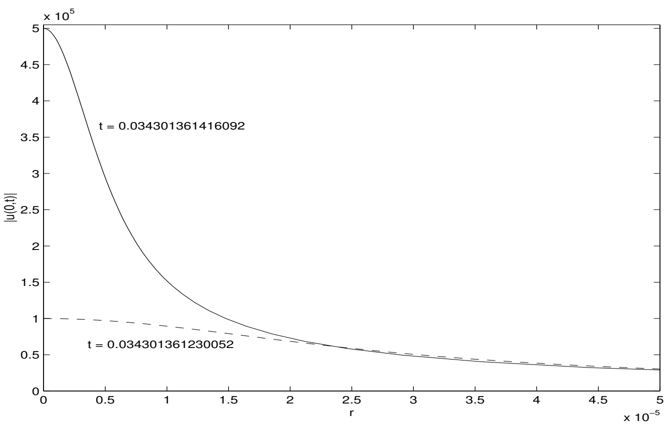

Figure 6.2: The solution when $|u(0,t)| = 100000$ and 500000

We now look at the mesh $X_i(t)$. If this is evolving in a self-similar manner then we would expect that $X_i(t) = \sqrt{T-t}\,Y_i$. Now, as $|u(0,t)| = Q(0)/\sqrt{(T-t)}$ then a self-similarly evolving solution and mesh should satisfy

$$X_i(t)|u(0,t)| = Q(0)Y_i.$$

Accordingly, in figure 6.3 we present a plot of $X_i(t)|u(0,t)|$ as a function of $\log(T-t)$ for a range in which u varies from 100 to 500000. Observe that these values rapidly evolve towards constants, demonstrating that the mesh is indeed evolving in a self-similar manner.

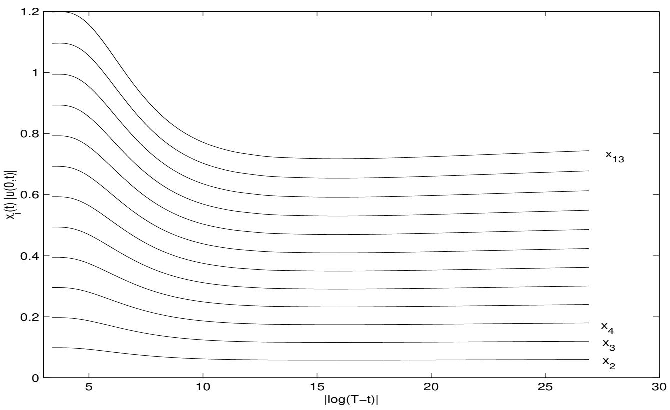

Figure 6.3: The scaled mesh $X_i(t)|u(0,t)|$

6.3 The linear heat equation

For our final calculation we consider the linear heat equation

$$u_t = u_{xx}, \tag{6.14}$$

on the bounded domain $x \in [0,1]$, with Dirichlet boundary conditions

$$u(0,t) = u(1,t) = 0, \tag{6.15}$$

and initial conditions approximating a Dirac measure. As was observed in Section 2, this problem may have an infinite number of different self-similar solutions and that the precise such solution may depend upon the time t. Thus we need to construct a numerical method invariant under the action of all such groups. As the heat equation has very stable solution patterns, we may (as in the case of the porous medium equation) use the mesh equation (4.13). The advantage of this is that it permits us to consider a wide class of monitor functions. This is necessary due to the many possible self-similar solutions admitted by this problem. For our monitor function we will consider the commonly used arc-length function

$$M = \sqrt{1 + u_x^2}. \tag{6.16}$$

As was observed earlier, this function is not scale invariant in general. However, if u_x is large, then M to a first approximation is given by $|u_x|$ which is scale invariant. We can regard arc-length as a regularisation of this function. When $|u_x|$ is small then arc-length reduces to 1 which is (trivially) scale invariant and leads to a uniform mesh. This is appropriate during the final evolution of the solution. This monitor function also has the advantage that it is not too much affected by the boundary conditions. Thus the mesh $X(\xi, t)$ must satisfy

$$\int_0^X \sqrt{1 + u_x^2}\, dx = \xi \int_0^1 \sqrt{1 + u_x^2}\, dx. \tag{6.17}$$

If $|u_x|$ is large and u has a single maximum then

$$\xi \int_0^1 \sqrt{1 + u_x^2}\, dx \approx 2\xi \max(u). \tag{6.18}$$

We now consider how the resulting continuous mesh behaves for solutions in the two asymptotic regimes described by (2.16) and (2.17). Consider first (2.16), in which we will assume that t is sufficiently small so that this self-similar description is appropriate. In this case we have

$$\int_0^X \frac{A}{\sqrt{t}} e^{-(x-x_0)^2/4t}\, dx = \xi \int_0^1 \frac{A}{\sqrt{t}} e^{-(x-x_0)^2/4t}\, dx$$

with u having a single maximum of $A/\sqrt{t} \gg 1$ at $x = x_0$. Now, as t is small, $|u_x|$ is large, apart from the immediate neighbourhood of the point x_0 and

$$\int_0^X \sqrt{1+u_x^2}\, dx \approx \int_0^X |u_x|\, dx \approx u(X) \quad \text{if} \quad X < x_0 \quad \text{or} \quad 2\max(u) - u(x) \quad \text{if} \quad X > x_0.$$

It follows from (6.18) that if we are close to the peak of the solution then

$$\frac{A}{\sqrt{t}} e^{(X-x_0)^2/4t} = \frac{2A}{\sqrt{t}} \xi \quad \text{if} \quad X < x_0,$$

and similarly

$$\frac{A}{\sqrt{t}} e^{(X-x_0)^2/4t} = \frac{2A}{\sqrt{t}} (1-\xi) \quad \text{if} \quad X > x_0.$$

The scaling invariance of the function $|u_x|$ has lead to the same factor of $A/\sqrt{t}$ arising in both sides of this equation and allows us to simplify and solve it. The resulting mesh is then given by

$$X(\xi,t) \approx x_0 - 2\sqrt{t}\sqrt{\log(1/2\xi)}, \quad \xi < 1/2, \tag{6.19}$$

$$X(\xi,t) \approx x_0 + 2\sqrt{t}\sqrt{\log(1/2(1-\xi))}, \quad \xi > 1/2. \tag{6.20}$$

(We have ignored here the behaviour very close to x_0 where u_x vanishes and M is very locally approximated by 1.)

Observe that this mesh automatically clusters points around the maximum at $x = x_0$ of the solution of the heat equation and that these points evolve in a correct self-similar manner consistent with the underlying scaling. Indeed, $X(\xi,t)$ evolves as

$$X(\xi,t) \approx x_0 + \sqrt{t}\, Y(\xi),$$

for some function $Y(\xi)$, the form of which follows from (6.19) and (6.20). There will be a small departure from scaling invariance in the immediate neighbourhood of the peak, but this may well be within a single mesh interval and will thus not affect the computation.

Now consider the next scaling range in which the boundary at $x = 0$ is important, but for which $1/\sqrt{t}$ is still large. Now from (2.17) we have that up to a constant

$$u(x,t) = \frac{Bx}{(t-t_0)^{3/2}} e^{-x^2/4(t-t_0)}. \tag{6.21}$$

We can rewrite this as

$$u(x,t) = \frac{B}{(t-t_0)} z e^{-z^2/4}, \quad z = x/\sqrt{t-t_0}$$

taking a maximum of $B\sqrt{2}e^{-1/2}/(t-t_0)$ when $z = \sqrt{2}$. When $(t-t_0)$ is small we can analyse the motion of the mesh in a similar manner to before. In particular, if $X/\sqrt{t-t_0} < \sqrt{2}$ then we have from the integration of the approximate monitor function $|u_x|$

$$f(Z) \equiv Z e^{-Z^2/4} = 2\xi\sqrt{2}e^{-1/2}, \quad \text{with} \quad Z = X/\sqrt{t-t_0}.$$

Thus

$$X(\xi,t) = \sqrt{t-t_0}\, f^{-1}\left(2\xi\sqrt{2}e^{-1/2}\right)$$

with $\xi = 1/2$ corresponding to $X = \sqrt{2(t-t_0)}$ and the function f^{-1} corresponding only to that part of the fuction $f(Z)$ on the interval $0 \leqslant Z \leqslant \sqrt{2}$. For $\xi > 1/2$ we have similarly that

$$X(\xi,t) = \sqrt{t-t_0}\, f^{-1}\left(2(1-\xi)\sqrt{2}e^{-1/2}\right)$$

where now f^{-1} corresponds to that part of the fuction $f(Z)$ on the interval $\sqrt{2} < Z < \infty$.

We see that in both cases we have again recovered a mesh which accurately picks up the correct self-similar form of the solution, with $X(\xi,t)$ evolving like $\sqrt{t-t_0}Y(\xi)$.

Thus the use of the monitor function based approach for this example has allowed the mesh to evolve in the correct self-similar manner in the two cases, even though the self-similar solution is taking two rather different forms. This example demonstrates the flexibility of our approach.

We present, in figure 6.4, some calculations of the evolution of the mesh obtained by solving the equation (6.17) in the regime for which we take u to be the self-similar solution (6.21). We see the mesh is initially scaling as $\sqrt{t}\,Y(\xi)$ close to $x = 0$ and eventualy becomes uniform as $u_x \to 0$ everywhere.

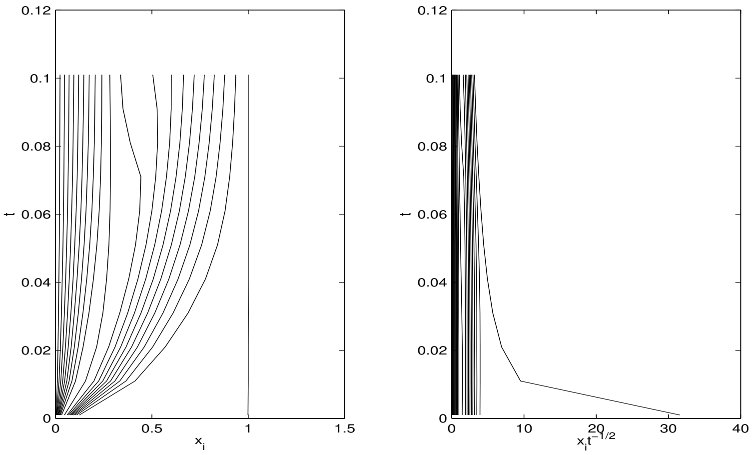

Figure 6.4: The mesh and scaled mesh for the second self-similar solution to the linear heat equation

7 Conclusions

We have shown in this review that scale invariant differential equations are common in many application areas and have interesting types of behaviour, with the form of the scaling underlying the solutions of the equations not always apparent at first inspection. Scale invariant adaptive numerical methods have the virtue of preserving many of the properties of such equations which are derived from their scaling, including their asymptotic behaviour. These methods do not, however, compromise the generality required of a numerical computational technique. The next stage of the work on these ideas is to develop them for problems which have scaling invariance in several spatial dimensions. This is the subject of our future work.

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