SCALING INVARIANCE AND ADAPTIVITY

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1 Introduction

Adaptivity is a commonly used tool for reducing computational costs when solving both partial and ordinary differential equations. Adaptive algorithms attempt to balance the local accuracy of a discrete approximation across space and/or time, so that the more difficult local approximations are performed using a finer mesh and/or timestep. A traditional and widely used form of adaptivity is to choose a step size so that some estimate of the truncation error error (obtained for example by using the Milne device [10],[11]) does not exceed a given bound over each discrete time interval. Whilst this approach is both powerful and flexible (and used in many commercial codes such as DDASSL [14]) it departs from the spirit of geometric integration in that it is not attempting (necessarily) to reproduce underlying qualitative structures in the solution. However, there is an alternative perspective on adaptivity which does this precisely. Suppose that a typical (autonomous) differential equation is

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u}), \tag{1.1}$$

where at this stage we won't be too precise about the function $\mathbf{f}(\mathbf{u})$. Now suppose that we consider the independent variable t to be itself a function of a *fictive* computational variable τ such that

$$\frac{dt}{d\tau} = g(\mathbf{u}); \tag{1.2}$$

then, under this Sundman transformation [12] the equation (1.1) transforms to

$$\frac{d\mathbf{u}}{d\tau} = g(\mathbf{u})\mathbf{f}(\mathbf{u}). \tag{1.3}$$

In any reasonable application we would seek to choose new coordinates so that the transformed equation (1.3) in the transformed variables (1.2) is in some ways easier to solve either analytically or numerically. In particular, singular solutions in the variable t should ideally become regular in the rescaled variable τ. Such a transformation may be made analytically and the resulting system (1.3) then solved numerically. We consider the advantages of this approach here. On the other hand, if we discretise (1.1) first and identify natural coordinates (1.2) *in the course of the calculation* then this process is at the heart of the adaptive approach. To see this we might suppose that in an adaptive procedure, we find an approximate solution to problem (1.1) at a series of discrete times t_n. Typically we would want $t_{n+1} - t_n$ to be small if some measure of the solution (such as the estimated local truncation error) is large. If we take $g(\mathbf{u})^{-1}$ to be this measure and $\Delta\tau$

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some prescribed tolerance, then a natural adaptive procedure for determining $t_{n+1} - t_n$ is to set

$$\Delta t_n \equiv t_{n+1} - t_n = \Delta\tau g(\mathbf{u}). \tag{1.4}$$

In the limit of small $\Delta\tau$ the equation (1.4) is simply a discretisation of the transformation implied by (1.2). This approach has been considered for Hamiltonian and reversible problems in the important paper [15] (see also [16]).

The choice of the function g in either the Sundman transformation (1.2) or the adaptive approach (1.4) is often somewhat arbitrary. However, in this paper we identify a class of problems for which there is a systematic way of finding a suitable function $g(\mathbf{u})$. These are differential equations of the form (1.1) which are invariant under the action of a *linear scaling group*. For partial differential equations describing physical phenomena, invariance of this nature is the norm rather than the exception and many examples are given in [1]. We show how the scaling function g can be determined *a-priori* for these differential equations by scaling arguments, making the condition that the transformed equation (1.3) should have the same scaling invariance as the original equation (1.1). In this case the resulting rescaled equations (1.4) can be discretised in a way which inherits the original scaling invariance. We also demonstrate that for this class an *a-posteriori* estimate of $g(\mathbf{u})$ in the formula (1.4) and related (and more sophisticated) adaptive formulae leads to essentially the same results, automatically identifying an appropriate fictive variable.

Both of the techniques of a-priori and a-posteriori scaling are effective in resolving singular structures especially when these structures have a self-similar form. We give evidence for this by looking at the solution of the Kepler problem under gravitational collapse. A similar approach has been developed for partial differential equations solved numerically using adaptive meshes [4], [5], [7], and many of the ideas of this paper translate easily into the context of a partial differential equation.

The structure of the remainder of this paper is as follows. In Section 2 we introduce the concept of a scale invariant system of ordinary differential equations and show how rescaling is coupled in a natural way to the invariance of the system (1.1) with respect to a linear Lie group. We identify a natural fictive variable τ by looking for complete invariance of the appropriately rescaled equations and show how the function $g(\mathbf{u})$ in the Sundman transformation can be derived. We then discuss the important class of self-similar solutions of the resulting equations which frequently describe singular behaviour. In Section 3 we consider multi-step and Runge-Kutta type discretisations of the Sundman transformed coupled systems (1.2),(1.3). In this section we demonstrate that the operations of discretisation and rescaling commute. This leads to excellent error control. Furthermore, we show that the schemes admit exact discrete self-similar solutions which *uniformly* approximate the true self-similar solutions over arbitrary long times and inherit the stability of these solutions. These results are presented in Theorem 3.3 and its Corollaries. In Section 4 we relate the a-priori Sundman transformation to a-posteriori adaptive methods based upon estimates of the relative local truncation error. In Section 5 we apply the methods developed to a series of scale invariant problems, considering both a-priori and a-posteriori scaling and looking at the special example of gravitational collapse. Finally in Section 6 we draw some conclusions from this work.

In a later paper we will address the issue of the interplay between scaling invariance and symplecticity in problems, such as the Kepler problem, which also have a Hamiltonian structure.

2 Rescaling, linear groups and adaptivity

We consider a particular class of ordinary differential equations, namely equations invariant under the action of a commutative linear scaling group. For such equations there is a very natural relation between scaling and an appropriate fictive coordinate τ. The invariance of physical equations under linear groups is universal and expresses the deep physics that the equations representing physical processes should not depend upon the units in which they are measured [1]. We show further that linear groups are unique amongst all group operations in that their action commutes both with discretisations of the differential equation and with coordinate transformations. Two examples of ordinary differential equations invariant under the action of rescaling are the blow-up equation,

$$\frac{du}{dt} = u^2,$$

and the motion of a particle in a one-dimensional gravitational field given by

$$\frac{d^2 r}{dt^2} = -\frac{1}{r^2}.$$

Both of these equations have solutions which develop singularities in a finite time, and the scaling invariance of the problem plays a significant role in describing this.

We show that scaling invariance of a system leads to a natural choice of the function g linking the time variable t with an appropriate fictive variable τ. Indeed we develop a simple calculus to enable such a procedure to be designed for a system of differential equations, provided that we know its scaling invariance. One of the nice features of this theory is that it works just as well for PDEs as for ODEs and is quite transparent for both. However, for clarity, we develop it here in the ODE context.

2.1 Linear invariance of a system of ordinary differential equations

We briefly review the theory of linear invariance in this section. For more details see [2], [8] or [13]. Consider the ordinary differential equation system

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u}), \quad \mathbf{u} = (u_1, u_2, .., u_N)^T, \quad \mathbf{f} = (f_1, f_2, .., f_N)^T. \tag{2.1}$$

It is immediate that that this system is invariant under the action of the affine transformation

$$t \to t + \lambda \quad \forall \lambda. \tag{2.2}$$

A *linear* rescaling transformation of the dependent and independent variables can be described by an $(N+1)$-tuple $\alpha = (\alpha_0, \alpha_1, ..., \alpha_N)$, such that if we introduce a rescaling parameter λ then the dependent and independent variables scale in the manner

$$t \to \lambda^{\alpha_0} t, \quad u_i \to \lambda^{\alpha_i} u_i, \quad \text{for all} \quad \lambda > 0. \tag{2.3}$$

A typical example of this would be a change in units of measurement, for example if u is a velocity and t is time, then scaling $t \to \lambda t$ induces a scaling of $u \to u/\lambda$. Clearly, a physical problem should not depend upon the units of measurement and this leads to the concept of scale invariance for a system of equations. Such a system (2.1) is invariant under the action of the rescalings (2.3) provided that for each i

$$\lambda^{\alpha_i-\alpha_0} f_i(u_1,..,u_N) = f_i(\lambda^{\alpha_1}u_1,..,\lambda^{\alpha_N}u_N). \tag{2.4}$$

It is quite possible (and is often the case) that there may be many such $(N+1)$-tuples α leaving (2.1) invariant. Indeed if α and α' are two such $(N+1)$-tuples then any linear combination corresponds to a further transformation, and all such transformations commute. Hence the set of all admissable transformations is equivalent to a vector space over R^{N+1}.

It is possible to identify a broad (but not exhaustive) class of function f_i which admit scaling invariant solutions. Differentiating (2.4) with respect to λ and setting $\lambda = 1$ we have

$$(\alpha_i - \alpha_0) f_i = \sum \alpha_j u_j \frac{\partial f_i}{\partial u_j}. \tag{2.5}$$

A general (though not complete) class of solution of this hyperbolic equation can be constructed as follows. For each i let

$$\beta_i = (\beta_{i,1}, \beta_{i,2}, .., \beta_{i,N})$$

be any N-vector such that

$$(\alpha_1, ..\alpha_N).\beta_i = 0,$$

and let

$$\gamma_{i,j} = (\gamma_{i,j,1}, \gamma_{i,j,2}, .., \gamma_{i,j,N})$$

be any set of J vectors, with $j = 1..J$ and J arbitrary, such that

$$(\alpha_1, .., \alpha_N).\gamma_i = p_i,$$

where p_i does not depend on j, and let μ_j be arbitrary constants. Then we may take

$$f_i = F_i(u_1^{\beta_{i,1}} u_2^{\beta_{i,2}}..u_N^{\beta_{i,N}}) \left[\sum_{j=1}^{J} \mu_j u_1^{\gamma_{i,j,1}} u_2^{\gamma_{i,j,2}}..u_N^{\gamma_{i,j,N}} \right]^{(\alpha_i-\alpha_0)/p_i}, \tag{2.6}$$

where F is an arbitrary function. In fact making simple changes we can take a product of similar function f_i to give a very wide class of admissable scale-invariant differential equations.

For a first example we take $N = 2, \alpha_0 = 1, \alpha_1 = 2$ and $\alpha_2 = 3$. Then for all i we can take $\beta_i = (3, -2)$. If furthermore we take $J = 1$ and supress dependence upon j we can take $\gamma_1 = (2, -1)$ and $\gamma_2 = (1, 0)$ with $p_1 = 1$ and $p_2 = 2$. Setting $(x, y) = (u_1, u_2)$ then give the system

$$\frac{dx}{dt} = x^2 y^{-1} F(x^3 y^{-2}), \quad \frac{dy}{dt} = x F(x^3 y^{-2}). \tag{2.7}$$

as invariant under the group action, where F and G are arbitrary functions.

As a second example we take $N = 2, \alpha_0 = 1, \alpha_1 = 2/3, \alpha_2 = -1/3, \alpha_3 = 2/3, \alpha_4 = -1/3$. Then we can take $\beta = 0$. Let $(x, u, y, v) = (u_1, u_2, u_3, u_4)$ then amongst the many possible systems invariant under this action we have

$$\frac{dx}{dt} = u, \quad \frac{du}{dt} = -\frac{x}{(x^2+y^2)^{3/2}}, \tag{2.8}$$

$$\frac{dy}{dt} = v, \quad \frac{dv}{dt} = -\frac{y}{(x^2+y^2)^{3/2}}. \tag{2.9}$$

This is the Kepler problem describing the two-dimensional motion of a particle under the gravitational attraction of a fixed mass. We note that this system also has the reflexional symmetry

$$t \to -t, \quad (x,y) \to (x,y), \quad (u,v) \to -(u,v), \tag{2.10}$$

and it is also invariant to any two-dimensional rotation.

2.2 Fully invariant rescalings of linearly invariant ODEs

Now consider Sundman type rescalings of invariant systems of ODEs introducing a fictive computational time variable τ so that

$$\frac{dt}{d\tau} = g(\mathbf{u}). \tag{2.11}$$

It is popular to choose g to equidistribute the local truncation error, arc-length or curvature of the solution. This choice can be somewhat arbitrary. We propose and consider here a more 'natural choice' of function derived from scaling arguments. Observe that g relates a fictive variable τ to a true variable t, so that when rescaled the dependent variable becomes a function of τ only. Now, suppose that this variable is changing rapidly with t. Such changes are, in the context we are considering ,*rescalings* of u and of t so that a change proportional to $\lambda^{\alpha_i} u_i$ in u_i should occur in a timescale proportional to λt. In the formation of a typical singularity governed by scaling structures there is often a finite time T such that as $t \to T$ some component in the solution $u_i \to \infty$. If at $t = T - \delta$ we have a solution u, then typically at time $t = T - \lambda\delta$ the solution becomes $\lambda^{\alpha_i} u_i$ with a singularity forming if $\alpha_i < 0$. Now suppose that we wish to compute this solution. To do this we would like to see such a process evolve in a continuous manner in the fictive time τ , so if for one fictive time interval $\Delta\tau$ we see changes Δu_i and δ in u_i and t respectively then in a similar fictive time interval $\Delta\tau$ we should see proportionally similar changes in the correspondingly rescaled values of u_i and t. This condition arises quite automatically if the following is satisfied:

The function g should be chosen such that the differential equation (2.11) is invariant under the action of the same symmetries as the original system of differential equations

Thus if t, u_i is a solution of (2.11) then so is $\lambda t, \lambda^{\alpha_i} u_i$ without having to rescale the independent variable τ.

The above condition leads to a procedure for calculating an admissable class of functions g and rejecting non-admissable functions. If we substitute the rescaled variables (2.3) into (2.11) we obtain

$$\lambda^{\alpha_0} g(u_1, .., u_N) = g(\lambda^{\alpha_1} u_1 ..., \lambda^{\alpha_N} u_N), \tag{2.12}$$

so on differentiating (2.12) with respect to λ and setting $\lambda = 1$ we have

$$\alpha_0 g = \sum \alpha_i u_i \frac{\partial g}{\partial u_i}. \tag{2.13}$$

This equation is very similar to that for each of the functions f_i in the previous section and has the same general solution (2.6) with each expression of the form $\alpha_i - \alpha_0$ replaced by one with α_0. However we should note that many functions, in particular arc-length, are not admitted by this formulation.

Suppose now that we have an ordinary differential equation with known symmetries. How do we choose an invariant function g amongst all of the possibilities? At this stage we should be guided by the paradigm that we should get the computer to do as much work as possible and that it is needless to over analyse the system to get an optimal scaling function g. Hence we argue for simplicity, indeed the results of the next section demonstrate that effectively all solutions of the equation (2.12) lead to essentially equivalent numerical schemes in terms of local error control and the admissability of discrete self-similar solutions.

A very simple such choice for the function g is

$$g = u_j^{\alpha_0/\alpha_j}, \tag{2.14}$$

where

$$|\alpha_j| = \max\{|\alpha_i|\}.$$

For the example (2.7) this gives $g = y^{1/3}$ so that on transforming the system we have

$$\frac{dx}{d\tau} = x^2 y^{-2/3} F(x^3 y^{-2}), \quad \frac{dy}{d\tau} = x y^{1/3} G(x^3 y^{-2}) \quad \frac{dt}{d\tau} = y^{1/3}. \tag{2.15}$$

For the Kepler problem (2.8),(2.9) we have

$$g = \frac{2}{3} x g_x + \frac{2}{3} y g_y - \frac{1}{3} u g_u - \frac{1}{3} v g_v. \tag{2.16}$$

If we set $r = \sqrt{x^2 + y^2}$ and suppose that $g \equiv g(r)$ then (2.16) reduces to

$$g = \frac{2}{3} r g_r,$$

so that

$$g = r^{3/2}. \tag{2.17}$$

We then have

$$x_\tau = r^{3/2} u, \quad u_\tau = -x/r^{3/2}, \quad y_\tau = r^{3/2} v, \quad v_\tau = -y/r^{3/2}, \quad t_\tau = r^{3/2}. \tag{2.18}$$

The discretisation of this system was studied in [3].

To summarise, the proposed invariant Sundman rescaling of (1.1) is given by

$$du_i/d\tau = g(\mathbf{u}) f_i(\mathbf{u}), \quad dt/d\tau = g(\mathbf{u}). \tag{2.19}$$

where g is any function satisfying the hyperbolic equation (2.13) such that

$$g(\lambda^{\alpha_1} u_1, \lambda^{\alpha_2} u_2, ..) f_i(\lambda^{\alpha_1} u_1, \lambda^{\alpha_2} u_2, ..) = \lambda^{\alpha_i} g(\mathbf{u}) f_i(\mathbf{u}), \tag{2.20}$$

and

$$g(\lambda^{\alpha_1} u_1, \lambda^{\alpha_2} u_2, ..) = \lambda^{\alpha_0} g(\mathbf{u}). \tag{2.21}$$

For convenience in further calculations we set

$$h_i(\mathbf{u}) = f_i(\mathbf{u})g(\mathbf{u}).$$

A nice feature of this rescaling is that it linearises scalar equations. Suppose that u and f are both scalars. Now set $h(u) = g(u)f(u)$. We have that $h(\lambda^\alpha u) = \lambda^\alpha h(u)$. As this must be true for all scalars λ we deduce that

$$h(u) = \beta u,$$

for some appropriate β, and hence

$$\frac{du}{d\tau} = \beta u,$$

linearising the differential equation.

We now investigate some of the properties of this rescaling and then look at discretisations of it.

2.3 Self-similar solutions

Most of the solutions of an invariant ordinary differential equation are (due to the prescription of arbitrary initial conditions) not themselves invariant under the action of the group. An important class of solutions do however have this property and are called *self-similar* solutions. Although such solutions are only admitted if the initial data satisfies certain algebraic constraints, they are often attractors for solutions with more general initial data and represent the long term asymptotics of the solution of the differential equation system. Self-similar solutions are especially important in the role that they play in describing singularity formation after the effects of initial conditions have decayed away. The ability of a method to accurately represent a similarity solution is an important test both for its ability to compute a singular solution and for it to represent the true long time asymptotics of the solution.

A general self-similar solution has the invariance

$$u_i(\lambda^{\alpha_0} t) = \lambda^{\alpha_i} u_i(t). \tag{2.22}$$

Differentiating with respect to λ and setting $\lambda = 1$ we obtain

$$\alpha_0 t \frac{du_i}{dt} = \alpha_i u_i,$$

so that

$$u_i = t^{\alpha_i/\alpha_0} u_i(1) \equiv u_i(t) = t^{\alpha_i/\alpha_0} U_i. \tag{2.23}$$

The values of the constants U_i are determined (up to an arbitrary scaling of the form $u_i \to \lambda^{\alpha_i} u_i$) by substituting (2.23) into the original differential equation to give the *algebraic* system

$$\alpha_i U_i = \alpha_0 f_i(\mathbf{U}), \quad \mathbf{U} = (U_1, U_2, ..., U_N). \tag{2.24}$$

Now, in the rescaled system (2.20) we also have

$$\frac{dt}{d\tau} = g(\mathbf{u}).$$

Thus,

$$\frac{dt}{d\tau} = g(t^{\alpha_i/\alpha_0}U_i) = tg(\mathbf{U}),$$

where the latter result follows from the scaling invariance of the function g. Without loss of generality we set $t = 1$ when $\tau = 0$. The self-similar solutions of (2.23) therefore have the form

$$t = \exp(\mu\alpha_0\tau), \quad u_i = U_i \exp(\mu\alpha_i\tau), \tag{2.25}$$

where we have that μ and $\mathbf{U}$ satisfy the algebraic system

$$\alpha_i\mu U_i = h_i(\mathbf{U}), \quad \alpha_0\mu = g(\mathbf{U}). \tag{2.26}$$

It is most significant that increasing the fictive time τ by a fixed amount $\Delta\tau$ corresponds precisely to a rescaling of the self-similar solution, so that each such increase in τ causes a proportionally similar increase in t and in u_i. This is exactly what makes this particular rescaling desirable from a computational viewpoint with τ as a fictive variable.

Applying this procedure firstly to problem (2.15) we have a self-similar solution of the form

$$x = Xe^{2\mu\tau}, \quad y = Ye^{3\mu\tau}, \quad t = e^{\mu\tau}.$$

So that on substituting, X, Y, μ satisfy the algebraic system

$$2\mu X = X^2Y^{-2/3}F(X^3Y^{-2}), \quad 3\mu Y = XY^{1/3}G(X^3Y^{-2}), \quad \mu = Y^{1/3}.$$

This implies that

$$3F(V) = 2G(V), \quad \text{where} \quad V = X^3Y^{-2}. \tag{2.27}$$

Assuming that this problem has a locally unique solution V then there is a one-parameter family of self-similar solutions given by

$$X = \lambda^2V^{1/3}, \quad Y = \lambda^3,$$

where λ is arbitrary.

For the rescaled Kepler problem (2.18) we have a self-similar solution of the form

$$x = Xe^{2\mu\tau/3}, \quad y = Ye^{2\mu\tau/3}, \quad u = Ue^{-\mu\tau/3}, \quad v = Ve^{-\mu\tau/3}, \quad t = e^{\mu\tau}.$$

Thus, X, Y, U, V, μ satisfy the algebraic system

$$\frac{2}{3}\mu X = (X^2+Y^2)^{3/4}U, \quad -\frac{1}{3}\mu U = -\frac{X}{(X^2+Y^2)^{3/4}},$$

with an almost identical equation for Y and V and

$$\mu = (X^2+Y^2)^{3/4}.$$

This has the solution

$$X = \left(\frac{9}{2}\right)^{1/3}, \quad U = \frac{2}{3}X, \quad \mu = \left(\frac{9}{2}\right)^{1/2}, \quad Y = V = 0. \tag{2.28}$$

Thus

$$(X^2+Y^2)^{3/2} = \frac{9}{2}.$$

and any plane rotation of this is also a solution. Now, observing the further symmetries $t \to T - t, \quad \tau \to -\tau, \quad x \to x, \quad u \to -u$, we also have a self-similar solution of the form

$$x = \left(\frac{9}{2}\right)^{1/3} e^{-2\mu\tau/3}, \quad u = -\frac{2}{3}\left(\frac{9}{2}\right)^{1/3} e^{\mu\tau/3}, \quad t = T - e^{-\mu\tau}. \tag{2.29}$$

which describes a gravitational collapse at time T.

It is interesting to compute the energy E of the self-similar solution. This is given by

$$E = \frac{1}{2}(u^2 + v^2) - \frac{1}{(x^2 + y^2)^{1/2}}. \tag{2.30}$$

This is a constant of the motion. Hence on a self-similar solution

$$E(\lambda^{2/3}x, \lambda^{2/3}y, \lambda^{-1/3}u, \lambda^{-1/3}v) = E(x, y, u, v).$$

But, by inspection from (2.30)

$$E(\lambda^{2/3}x, \lambda^{2/3}y, \lambda^{-1/3}u, \lambda^{-1/3}v) = \lambda^{-2/3}E(x, y, u, v).$$

As λ is arbitrary, E can only be constant if it is zero. Thus without explicitly calculating E for the self-similar solution we can deduce that it is zero.

3 Some Properties of the discretisations of scale invariant ODEs

In this section we consider discretising the Sundman transformed system (2.19) using a variety of methods. Although this system is slightly more complex than the original system (1.1), solving the new system has distinct advantages over discretising the original. We identify three such advantages.

1. Multi-step discretisations of (2.19) have local truncation errors which are independent of scale.
2. Any continuous self-similar solutions are uniformly (in time) approximated by exact discrete self-similar solutions.
3. Global properties of the solution which are derived from scaling invariance (an example being Kepler's third law for planetary motion) are automatically inherited by the numerical method.

All of these observations follow from the fact that the two operations of linear scaling and discretisation *commute* when applied to (2.19). We now demonstrate this.

3.1 The commuting of scaling and discretisation

The rescaled problem is to find $\mathbf{u}(\tau)$ and $t(\tau)$ such that

$$d\mathbf{u}/d\tau = \mathbf{f}(\mathbf{u})g(\mathbf{u}) \equiv \mathbf{h}(\mathbf{u}), \quad dt/d\tau = g(\mathbf{u}), \tag{3.1}$$

where, as a consequence of the choice of the function g

$$\mathbf{h}(..., \lambda^{\alpha_i} u_i, ...) = \lambda^{\alpha_i} \mathbf{h}(u_i), \quad g(..., \lambda^{\alpha_i} u_i, ...) = \lambda^{\alpha_0} g(\mathbf{u}). \tag{3.2}$$

Consider first a linear multi-step discretisation of (3.1) so that

$$\mathbf{u}_n \equiv (u_{1,n}, u_{2,n}, ..., u_{i,n}) \approx \mathbf{u}(n\Delta\tau), \quad t_n \approx t(n\Delta\tau),$$

are approximations to $\mathbf{u}$ and t with $\Delta\tau$ fixed. Now, for appropriate β_j and γ_j set

$$\sum_{j=0}^{l} \beta_j \mathbf{u}_{n-j} = \Delta\tau \sum_{j=0}^{l} \gamma_j \mathbf{h}(\mathbf{u}_{n-j}) \quad \sum_{j=0}^{l} \beta_j t_{n-j} = \Delta\tau \sum_{j=0}^{l} \gamma_j g(\mathbf{u}_{n-j}). \tag{3.3}$$

It is immediate, on inspection of (3.3), that if $(t_n, u_{i,n})$ is a solution of (3.3) for $n = 0, 1, ...$ then so is the rescaled solution $(\lambda^{\alpha_0} t_n, \lambda^{\alpha_i} u_{i,n})$. All we have to do is substitute the latter expression in to (3.3), and exploit the scaling structure of the functions f_i and g.

Hence the linear multi-step method (with a fixed step size $\Delta\tau$) inherits exactly the same scaling invariance as the original system. This is quite a deep result. We are saying that the two operations of scaling and discretisation when applied to a differential equation system *commute*. This result is simply not true when applied to a fixed step (non-adaptive method). It is implicit in the rescaling that the time step Δt can be rescaled along with the solution. If this is not done then rescaling in time is simply not possible.

The property that rescaling and discretisation commute is one which applies only to a linear or affine transformation and not for a more general map. To see this we consider the simplest one-dimensional problem

$$\frac{du}{dt} = f(u), \tag{3.4}$$

and rescale this under the map

$$u = a(v) \tag{3.5}$$

to give

$$\frac{dv}{dt} = \frac{f(a(v)))}{a'(v)}. \tag{3.6}$$

Now, consider a linear multi-step discretisation of (3.4) giving

$$\sum_{j=0}^{l} \beta_j u_{n-j} = \Delta t \sum_{j=0}^{l} \gamma_j f(u_{n-j}). \tag{3.7}$$

Applying the rescaling transformation (3.5) to the discrete system (3.7) we have

$$\sum_{j=0}^{l} \beta_j a(v_{n-j}) = \Delta t \sum_{j=0}^{l} \gamma_j f(a(v_{n-j})). \tag{3.8}$$

Alternatively, applying the multi-step discretisation to the rescaled system (3.6) gives

$$\sum_{j=0}^{l} \beta_j v_{n-j} = \Delta t \sum_{j=0}^{l} \gamma_j \frac{f(a(v_{n-j}))}{a'(v_{n-j})}. \tag{3.9}$$

The two expressions (3.8) and (3.9) will in general not be the same. If Δt is small, then a simple calculation indicates that the difference between them is proportional to

$$(\Delta t)^2 \left[a^{-1}(v)\right]''.$$

Hence, (3.8) and (3.9) can only agree in this limit if

$$(\Delta t)^2 \left[a^{-1}(v)\right]'' = 0,$$

so that $a(v)$ has to be the affine transformation

$$a(v) = \mu + \lambda v.$$

This is of course a necessary condition. However, it follows from the consistency of the method ie. $\sum \beta_j = 0$ that this condition is also sufficient. A similar result holds also for transformations of the dependent variable.

If we use instead a Runge-Kutta discretisation of the system as given by

$$\begin{aligned}
\xi_n^j &= \mathbf{u}_n + \Delta\tau \sum_{l=1}^{\nu} a_{j,l}\mathbf{h}(\xi_n^l), \quad j = 1 \ldots \nu, \\
\mathbf{u}_{n+1} &= \mathbf{u}_n + \Delta\tau \sum_{j=1}^{\nu} b_j \mathbf{h}(\xi_n^j), \\
t_{n+1} &= t_n + \Delta\tau \sum_{j=1}^{\nu} b_j g(\xi_n^j),
\end{aligned}$$

then it is simple to show that the rescaling $(\lambda^{\alpha_0} t_n, \lambda^{\alpha_i} u_{i,n})$ is also an admissable solution. The result follows from (3.2) after substituting the rescaled solution and the fact that intermediate steps scale as $\lambda^{\alpha_i}\xi_{i,n}^j$, which is exactly what we want and expect.

The global properties of the solution derived from scaling invariance follow immediately from the invariance of the numerical method. For example, suppose that (x, y) is a periodic solution of the Kepler problem with period T, then Kepler's third law states that the square of the period is proportional to the cube of the major axis of the orbit. This is equivalent to saying that given the above periodic solution, the orbit $(\lambda^2 x, \lambda^2 y)$ is also a solution with period $\lambda^3 T$, and this is precisely a statement of scaling invariance. Now suppose that (x_n, y_n) is a discrete periodic solution with period T_Δ, then immediately from the invariance of the numerical scheme, $(\lambda^2 x_n, \lambda^2 y_n)$ is also a discrete periodic solution with period $\lambda^3 T_\Delta$, and hence Kepler's law holds in the discrete case.

3.2 Local truncation error of the multi-step method

We show in this subsection that the relative error in a linear multi-step discretisation is independent of scale. As the errors in such discretisations involve higher derivatives of $\mathbf{u}$ we must firstly determine the way that these derivatives scale themselves. This is given by the following theorem

THEOREM 3.1 *The n-th derivatives* $u_i^{(n)}$ *of the components of* $\mathbf{u}$ *with respect to* τ *satisfy the equations*

$$u_i^{(n)} = h_i^{(n)}(\mathbf{u}), \tag{3.10}$$

where the functions $h_i^{(n)}$ *have the scaling law*

$$h_i^{(n)}(..., \lambda^{\alpha_j} u_j, ...) = \lambda^{\alpha_i} h_i^{(n)}(\mathbf{u}). \tag{3.11}$$

Here we have that $h_i^{(0)} \equiv h_i$ and we see that each of the subsequent functions $h_i^{(n)}$ scales in an identical manner to h_i.

Proof The proof is by induction on n. Clearly the result is true if $n = 1$. Now differentiate the expression (3.10) with respect to τ to give

$$u_i^{(n)} = \frac{du_i^{(n)}}{d\tau} = \sum_k \frac{\partial h_i^{(n)}}{\partial u_k} \frac{du_k}{d\tau} = \sum_k \frac{\partial h_i^{(n)}}{\partial u_k} h_k \equiv h_i^{(n+1)}.$$

Thus

$$h_i^{(n+1)}(.., \lambda^{\alpha_j} u_j, ..) = \sum_k \frac{\partial h_i^{(n)}}{\partial u_k}(.., \lambda^{\alpha_j} u_j, ..) h_k(.., \lambda^{\alpha_j} u_j, ..).$$

But differentiating the identity (3.11) with respect to u_k gives

$$\frac{\partial h_i^{(n)}}{\partial u_k}(.., \lambda^{\alpha_j} u_j, ..) = \lambda^{\alpha_i - \alpha_k} \frac{\partial h_i^{(n)}}{\partial u_k}(\mathbf{u}).$$

Hence

$$h_i^{(n+1)}(.., \lambda^{\alpha_j} u_j, ..) = \sum_k \lambda^{\alpha_i - \alpha_k} \frac{\partial h_i^{(n)}}{\partial u_k}(\mathbf{u}) \lambda^{\alpha_k} h_k(\mathbf{u}) = \lambda^{\alpha_i} h_i^{(n+1)}(\mathbf{u}),$$

and the result follows.

Thus all of the derivatives of u_i with respect to τ scale in exactly the same manner as u_i itself. In particular, each of the expressions of the relative derivative

$$v_i^{(n)} \equiv \frac{u_i^{(n)}}{u_i}$$

is invariant under rescaling.

Now consider the multi-step method of order p (3.3). From the standard theory of such methods [10], [11], it follows that the local truncation error $\mathbf{e}$ is given by

$$\mathbf{e} = C(\Delta\tau)^{p+1} \mathbf{u}^{(p+1)} + \mathcal{O}(\Delta\tau^{p+2}),$$

where C is a constant. To leading order the relative error contributions are given by

$$\frac{e_i}{u_i} = C(\Delta\tau)^{p+1} \frac{u_i^{(p+1)}}{u_i}.$$

From the above reasoning we see that these are invariant under rescaling. Thus if we define the relative local truncation error to be

$$E = \max_i (e_i/u_i),$$

then for a method with constant step-size $\Delta\tau$ this error is also invariant under rescaling.

It is hard to over emphasise the importance of this result. If a singularity forms in the solution which is progressivley described in terms of the action of the scaling group, then the resulting adaptive numerical method will continue to compute this solution with no overall loss of relative accuracy. We will see this clearly demonstrated when we look at the problem of gravitational collapse.

Observe, however, that an overall error defined by $\|\mathbf{e}\|$ is not invariant under rescaling, and indeed has no nice scaling properties.

3.3 Admittance of discrete self-similar solutions

A key feature of both the multi-step and Runge-Kutta discretisations of the invariant schemes, is that they are able to approximate the self-similar manifold for all time to a constant discretisation error which does not grow with increasing τ even if the solution forms a singularity.

To state our main result, consider the original scale invariant problem

$$\dot{u}_i = f_i(\mathbf{u}), \tag{3.12}$$

with the self-similar solution

$$u_i(t) = U_i t^{\alpha_i/\alpha_0} \tag{3.13}$$

The constants U_i then satisfy the *algebraic* system

$$\alpha_i U_i = \alpha_0 f_i(\mathbf{U}) \quad \text{where} \quad \mathbf{U} = (U_1, U_2, ..)^T. \tag{3.14}$$

From (2.25) we have that the general self-similar solution to (2.19) is given by

$$u_i = U_i e^{\mu\alpha_i\tau}, \quad t = e^{\mu\alpha_0\tau}, \tag{3.15}$$

where, if without loss of generality we set $t = 1$ at $\tau = 0$ then

$$\mu = g(\mathbf{u})/\alpha_0.$$

We consider first using the linear multi-step method (3.3) to solve (2.19). The following lemma is an immediate consequence of the scaling invariance of the multi-step method

LEMMA 3.2 *If $u_{i,n}$ and t_n are discrete approximants to u_i and t then, for suitable constants $\hat{U}_i$ and z satisfying an appropriate nonlinear equation, there is a discrete self-similar solution of the form*

$$u_{i,n} = \hat{U}_i z^{\alpha_i n}, \quad t_n = z^{\alpha_0 n}. \tag{3.16}$$

which is valid for all $n \geqslant 0$. For this solution it is immediate that

$$u_{i,n} = \hat{U}_i t_n^{\alpha_i/\alpha_0}. \tag{3.17}$$

Proof The proof of this result is almost immediate. Observe that from (2.19)

$$h_i(.., \hat{U}_k z^{\alpha_k(n-j)}, ..) = z^{(n-j)\alpha_i} h_i(.., \hat{U}_k, ..).$$

Thus the expression (3.16) satisfies the linear multi-step method (3.3) provided that for all i we have

$$\sum_j \beta_j z^{(n-j)\alpha_i} \hat{U}_i = \Delta\tau \sum_j z^{(n-j)\alpha_i} \gamma_j h_i(\hat{\mathbf{U}}),$$

and

$$\sum_j \beta_j z^{(n-j)\alpha_i} \hat{U}_i = \Delta\tau \sum_j z^{(n-j)\alpha_i} \gamma_j g(\hat{\mathbf{U}}).$$

Most significantly, this system is satisfied for all values of n provided that $\hat{U}_i$ and z satisfy the follwing nonlinear algebraic system

$$\sum_j \beta_j z^{-j\alpha_i} \hat{U}_i - \Delta\tau \sum_j \gamma_j z^{-j\alpha_i} h_i(\hat{\mathbf{U}}) = 0, \tag{3.18}$$

and

$$\sum_j \beta_j z^{-j\alpha_0} - \Delta\tau \sum_j \gamma_j z^{-j\alpha_0} g(\hat{\mathbf{U}}) = 0. \tag{3.19}$$

We now proceed to show that (3.18),(3.19) has a solution in a sense close to the underlying self-similar solution.

THEOREM 3.3 *Suppose that the self-similar solution (3.15) exists and is locally unique. Suppose furthermore that the linear multi-step method has a local truncation error which is of order $\mathcal{O}\left(\Delta\tau^{p+1}\right)$, then for sufficiently small $\Delta\tau$ the system (3.18),(3.19) has a locally unique solution satisfying*

$$\hat{U}_i = U_i + \mathcal{O}\left(\Delta\tau^p\right), \tag{3.20}$$

$$z = e^{\mu\Delta\tau} + \mathcal{O}\left(\Delta\tau^{p+1}\right). \tag{3.21}$$

CORROLLARY 3.4 *For all time it follows that*

$$\frac{u_{i,n}}{t_n^{\alpha_i/\alpha_0}} = \frac{u_i(t_n)}{t_n^{\alpha_i/\alpha_0}} + \mathcal{O}\left(\Delta\tau^p\right), \tag{3.22}$$

where the implied constant in the $\mathcal{O}$ term does not depend upon either the solution or on t.

The proof of this result follows from an application of the Implicit Function Theorem. Consider the true self similar solution given by (3.15). If we set $x = \exp(\mu\Delta\tau)$ we have immediately that

$$u_i(j\Delta\tau) = U_i x^{j\alpha_i}, \quad t(j\Delta\tau) = x^{j\alpha_0}.$$

Hence, substituting into the Linear Multi-step scheme (3.3), exploiting the scaling properties of the scheme and looking at the local truncation error we have

$$\sum_j \beta_j x^{-j\alpha_i} U_i - \Delta\tau \sum_j \gamma_j x^{-j\alpha_i} h_i(\mathbf{U}) = \mathcal{O}\left(\Delta\tau^{p+1}\right), \tag{3.23}$$

$$\sum_j \beta_j x^{-j\alpha_0} - \Delta\tau \sum_j \gamma_j x^{-j\alpha_i} g(\mathbf{U}) = \mathcal{O}\left(\Delta\tau^{p+1}\right), \tag{3.24}$$

Thus $(\mathbf{U}, x)$ is an approximate solution of (3.20),(3.21) with an error of $\mathcal{O}\left(\Delta\tau^{p+1}\right)$. Now, to be a self-similar solution the values U_i must satisfy the nonlinear algebraic equations

$$\mu\alpha_i U_i - h_i(\mathbf{U}) = 0, \quad \mu\alpha_0 - g(\mathbf{U}) = 0. \tag{3.25}$$

Thus the continuous self-similar solution is locally unique provided that the Jacobian matrix J defined by

$$J = \left[\begin{array}{c|c} \alpha_i U_i & \mu\alpha_i\delta_{i,j} - \partial h_i/\partial U_j \\ \hline \alpha_0 & -\partial g/\partial U_j \end{array}\right] \tag{3.26}$$

(where $\delta_{i,j}$ is the Kronecker delta) has a bounded inverse. Now consider the Jacobian of the operator defined by the left hand side of the equation (3.23), (3.24). We define the polynomial $a(z)$ by

$$a(z) = \sum_j \beta_j z^{-j}$$

and note that for consistency and zero-stability of the multi-step scheme we must have

$$a(1) = 0, \quad a'(1) \neq 0.$$

Furthermore, we observe from the definition of x that for small $\Delta\tau$ we have

$$x = 1 + \mu\Delta\tau + \mathcal{O}\left(\Delta\tau^2\right),$$

so that

$$a(x^{\alpha_i}) = a'(1)\Delta\tau\alpha_i\mu + \mathcal{O}\left(\Delta\tau^2\right).$$

Combining these results, it follows immediately that the Jacobian of the nonlinear system (3.18), (3.19) is given by J_Δ where

$$J_\Delta = a'(1)\left[\begin{array}{c|c} \alpha_i U_i + \mathcal{O}(\Delta\tau) & \Delta\tau(\mu\alpha_i\delta_{i,j} - \partial h_i/\partial U_j) + \mathcal{O}(\Delta\tau^2) \\ \hline \alpha_0 + \mathcal{O}(\Delta\tau) & -\Delta\tau\partial g/\partial U_j + \mathcal{O}(\Delta\tau^2) \end{array}\right]. \tag{3.27}$$

Now suppose that we rescale the system (3.23),(3.24) by setting $\hat{U}_i = U_i + \delta_i/\Delta\tau, \quad z = x + \delta z$ The Jacobian of the resulting rescaling acting on the vector $[\delta z, \delta_i]$ is given by

$$\hat{J}_\Delta = a'(1) \left[\begin{array}{c|c} \alpha_i U_i & \mu\alpha_i\delta_{i,j} - \partial h_i/\partial U_j \\ \hline \alpha_0 & -\partial g/\partial U_j \end{array} \right] + \mathcal{O}(\Delta\tau)$$

$$= a'(1)J + \mathcal{O}(\Delta\tau),$$

where J is the matrix given in (3.26). Now, as J has a bounded inverse, it follows that in the limit of small $\Delta\tau$ the matrix $\hat{J}_\Delta$ also has a bounded inverse in this limit. Hence we can apply the implicit function theorem to (3.23),(3.24) to find a solution. This gives

$$[\delta z, \delta_i] = \mathcal{O}(\Delta\tau^{p+1}).$$

Thus

$$z = x + \mathcal{O}\left(\Delta\tau^{p+1}\right), \quad \hat{U}_i = U_i + \mathcal{O}\left(\Delta\tau^{p}\right),$$

and the theorem follows.

It is not difficult to show, using an almost identical method of proof that the same results as stated in Theorem 3.3 and Corollary 3.4 holds for the Runge-Kutta method described earlier.

Having established that we approximate the manifold geometry of the self-similar solutions with a *uniform* accuracy for all time we now turn our attention to looking at (i) the dynamics on this manifold (ii) the dynamics close to the manifold.

3.3.1 The dynamics on the self-similar manifold

We have that

$$z = e^{\mu\Delta\tau} + \mathcal{O}\left(\Delta\tau^{p+1}\right),$$

and that at the fictive time $n\Delta\tau$

$$t_n = z^{\alpha_0 n}, \quad t = e^{n\mu\alpha_0\Delta\tau}.$$

Thus at this fictive time

$$t_n = \left[e^{\mu\Delta\tau} + \mathcal{O}(\Delta\tau^{p+1})\right]^{\alpha_0 n} = e^{n\mu\alpha_0\Delta\tau}\left[1 + \mathcal{O}(n\Delta\tau^{p+1})\right].$$

Now $\log(t) = n\mu\Delta\tau$ and hence

$$t_n/t = 1 + \mathcal{O}(\Delta\tau^p \log(t)). \tag{3.28}$$

So, the relative error in t_n (and hence in each of the terms $u_{n,i}$) grows very slowly for large t.

Of course, in a sense this is a fictional error which is introduced due to our use of a fictive time and the fact that we are making comparisons at the same fictive time. As an alternative (and more realistic) measure of the error we can compare $u_{n,i}$ with u_i at the same real time t_n. The following result follows immediately

COROLLARY 3.5

$$u_i(t_n)/u_{n,i} - 1 = U_i/\hat{U}_i - 1 = \mathcal{O}(\Delta\tau^p).$$

Proof This follows immediately from the result

$$u_i(t_n) = U_i t_n^{\alpha_i/\alpha_0} \quad \text{and} \quad u_{n,i} = \hat{U}_i t_n^{\alpha_i/\alpha_0}.$$

3.3.2 The dynamics close to the self-similar manifold

Now consider the dynamics close to the manifold. For a general system with general initial conditions, the self-similar solutions, though invariants of the system, do not satisfy the initial conditions. However, it is frequently the case that such solutions are often attractors and it is desirable that the numerical method should preserve this structure.

The general form of the perturbation to a self-similar solution such as (2.25) takes the form

$$u_i(\tau) = e^{\mu\alpha_i\tau}\left[U_i + a_i\right], \quad t(\tau) = e^{\mu\alpha_0\tau}\left[1 + s\right]. \tag{3.29}$$

Where, using the scaling invariance of the functions, we have to leading order

$$\dot{a}_i + \mu\alpha_i a_i = \sum \frac{\partial h_i}{\partial u_j} a_j, \quad \dot{s} + \mu\alpha_0 s = \sum \frac{\partial g}{\partial u_j} a_j. \tag{3.30}$$

In general this system will have solutions of the form

$$a_i = A_i e^{\kappa_k\tau}, \quad s = S e^{\kappa_k\tau}, \tag{3.31}$$

where

$$\kappa_k A_i + \mu\alpha_i A_i = \sum \frac{\partial h_i}{\partial u_j} A_j, \quad \kappa_k s + \mu\alpha_0 s = \sum \frac{\partial g}{\partial u_j} A_j. \tag{3.32}$$

and we have eigenvalues $\kappa_k, \quad k = 1..N+1$. The solutions of this eigenvalue problem then determine the stability of the self-similar solution. We observe immediately that there are two solutions to this problem which can be obtained from scaling arguments. The first follows from the observation that we may make an arbitrary perturbation to τ of the form $\tau \to \tau + \varepsilon$. This is equivalent to a rescaling of the original self-similar solution and corresponds to taking

$$\kappa_1 = 0, \quad A_i = \varepsilon\mu\alpha_i U_i, \quad S = \varepsilon\mu\alpha_0.$$

The second follows from the observation that the original equation (1.1) is invariant under the action of $t \to t + \varepsilon$ and this corresponds to taking

$$\kappa_2 = -\mu\alpha_0, \quad A_i = 0, \quad S = \varepsilon.$$

For stability we require that $Re(\kappa_k) < 0$ for all $k > 2$.

Now consider the discrete self-similar solution. A perturbation to this takes the form

$$u_{i,n} = z^{\alpha_i n}\left[\hat{U}_i + \hat{a}_{i,n}\right], \quad t_n = z^{\alpha_0 n}\left[1 + \hat{s}_n\right]. \tag{3.33}$$

Arguing in a similar manner to before we may pose a solution of (3.33) of the form

$$\hat{a}_i = \hat{A}_i z^{\nu_k n}, \quad \hat{s} = \hat{S} z^{\nu_k n} \tag{3.34}$$

Because the same symmetries are acting on the discrete and continuous systems we may deduce, in a similar manner to before, that there are two eigenmodes with corresponding eigenvalues:

$$\nu_1 = 0, \quad \text{and} \quad \nu_2 = -\alpha_0.$$

Stability follows if $\nu_k < 0$ if $k > 2$. Substituting (3.34) into the discretised equation and applying Theorem 3.3 we have (after some manipulation) that the eigenvalue equation satisfied by the terms ν_k is (up to a rescaling) identical to that satified by the eigenvalues κ_k up to a discretisation error of $\mathcal{O}(\Delta\tau^p)$. Hence (up to a rescaling) the eigenvalues ν_k are (noting the equality of the eigenvalues when $k = 1$) perturbations of the eigenvalues κ_k. Hence, for small $\Delta\tau$ stability of the true self-similar solution implies stability of the discrete self-similar solution. We shall see this when we consider the numerical examples in Section 5.

4 Adaptivity and rescaling

4.1 Adaptivity for ordinary differential equation methods

We consider now the relation between adaptivity and rescaling. The previous sections have shown that a discretisation of an appropriately rescaled equation has many desirable properties. We may ask the converse question: given a differential equation with scaling invariance, can the method automatically identify a suitable rescaling. We now demonstrate that this does follow provided a suitable adaptive strategy is used.

Consider a linear multi-step discretisation of the original problem (1.1) of the form

$$\sum_j \beta_j \mathbf{u}_{n-j} = \Delta t_n \sum_j \gamma_j \mathbf{f}(\mathbf{u}_{n-j}). \tag{4.1}$$

A typical adaptive numerical method, aims to construct a sequence of solution approximations u_n at times t_n where $\Delta t_n \equiv t_{n+1} - t_n$ is chosen in some appropriate manner.

A common device for determining Δt_n is to make some estimate of the error and to then choose Δt_n so that this estimate is bounded over each time interval.

As a first estimate we consider the relative local trunction error of the method defined in a similar way to (3.3). Again following [10], [11], the local truncation error is given to leading order by

$$\mathbf{e} = C\Delta t_n^{p+1}\mathbf{u}^{(p+1)},$$

where for this section we consider all derivatives of $\mathbf{u}$ as derivatives in t. Following the previous section we now consider the relative local trunction error

$$E(\Delta t_n) = \max |e_i/u_i|.$$

Assuming for the present that we can estimate this error term, then we can choose Δt_n to bound it. Provocatively we set this upper bound to be $(\Delta\tau)^{p+1}$ for some fixed $\Delta\tau$. One method of calculating Δt_n is to thus set

$$E(\Delta t_n) = \Delta\tau^{p+1}, \tag{4.2}$$

and to solve the equation (4.2) for Δt_n. Using the estimate for E and setting all constants to unity, we thus have

$$\Delta t_n = \Delta\tau \left(\min |u_i / u_i^{(p+1)}| \right)^{1/(p+1)} \equiv \Delta\tau g(\mathbf{u}). \tag{4.3}$$

We now observe that in the limit of small $\Delta\tau$ the equation (4.3) is precisely a leading order discretisation of the ordinary differential equation

$$\frac{dt}{d\tau} = g(\mathbf{u}).$$

Now consider how the function $g(\mathbf{u})$ scales. A very similar calculation to that presented in the last section gives that under the rescaling (2.3) we have that

$$u_i^{(p+1)}(\lambda^{\alpha_0} t) \to \lambda^{\alpha_i - (p+1)\alpha_0} u_i^{(p+1)}(t).$$

Hence from the definition of g

$$g(.., \lambda^{\alpha_i} u_i, ..) \to \left(\min \left(\frac{\lambda^{\alpha_i}}{\lambda^{\alpha_i - (p+1)\alpha_0}} g(\mathbf{u}) \right) \right)^{1/(p+1)} = \lambda^{\alpha_0} g(\mathbf{u}).$$

Thus the function g derived from the relative local truncation error estimate scales in precisely the manner required by the function specified in Section 2 so that the resulting equation for $\mathbf{u}$ in terms of τ is scale invariant.

Thus the results of the previous two sections apply immediately to this case. Observe however, that the discretisation implied by this adaptive approach is only first order accurate, thus whilst it will follow a self-similar solution it may (though not necessarily) do so at a reduced level of accuracy.

Of course in practice the local truncation error is not available to us and it must be estimated. Moreover it is generally hard to solve (4.2) exactly for Δt_n, and instead Δt_n is often succesively halved until $E(\Delta t_n)$ or some other error measure is bounded above by $\Delta\tau^{p+1}$. One such method is to use the Milne device [10], [11] in which two computations of an approximate solution are made using two different multi-step methods, and the difference between them used as an estimate of the error E. In principle, provided the leading order behaviour of the error accurately reflects the true error, then the estimate for E based upon the Milne device will have exactly the same scaling properties as the above estimate. Thus if E is estimated by this manner and (4.2) solved, the resulting method will be scale invariant. It is unclear, at this stage, what the precise effect on the scale invariance will be on instead succesively halving Δt_n till $E(\Delta t_n) < \Delta\tau^{p+1}$ and we leave this as a subject for further research.

It is interesting to also look at error control based upon equidistributing some other measure of the solution. A popular such measure [9] is the arc-length of the solution.

In the context of a continuous adaptive method this would imply that we would take Δt_n so that

$$\sqrt{1+|\mathbf{u}_t|^2}\Delta t_n = \Delta\tau,$$

and hence the appropriate function $g(\mathbf{u})$ is given by

$$g(\mathbf{u}) = \frac{1}{\sqrt{1+|\mathbf{u}_t|^2}}.$$

Such methods do not fit easily into our framework as the arc-length function does not scale in any meaningful way under the rescaling transformations. For example, if $\mathbf{u}_t$ is large then the arclength is approximated by $\max(u_{i,t})$ in which case under rescaling we have

$$g \to \max(\lambda^{\alpha_i-\alpha_0})g.$$

It should be emphasised that arc-length has certain advantages when used for Hamiltonian problems, and some of these are discussed in [9].

5 Numerical examples

We consider three examples in this section to illustrate the results of the previous section. The first is a simple one to illustrate the use of a-priori scaling. The second we look at a-posteriori scaling. In the third we look at the singular problem of gravitational collapse.

Example 1 A-priori scaling.

Consider the simple system

$$\frac{du}{dt} = u^{-2}. \tag{5.1}$$

This has the scale invariance

$$t \to \lambda t, \quad u \to \lambda^{1/3}u$$

so that

$$\alpha_0 = 1, \quad \alpha_1 = 1/3.$$

Is has the self similar solution.

$$u = (3t)^{1/3}. \tag{5.2}$$

To give an invariant formulation of (5.1) we solve the hyperbolic equation

$$\frac{1}{3}ug_u = g$$

so that

$$g = u^3.$$

The Sundman transformation then leads to the invariant system

$$\frac{du}{d\tau} = u, \quad \frac{dt}{d\tau} = u^3 \tag{5.3}$$

with the self-similar solution

$$u = 3^{1/3}e^{\tau}, \quad t = e^{3\tau}. \tag{5.4}$$

so that $\mu = 3$ in equation (2.25). Observe that this transformation has linearised the equation for u. If we discretise the system (5.3) using the Trapezoidal rule with constant step size $\Delta\tau$ with (u_n, t_n) approximations for $(u(n\tau), t(n\tau))$ we obtain

$$u_{n+1} - u_n - \frac{\Delta\tau}{2}(u_n + u_{n+1}) = 0, \tag{5.5}$$

and

$$t_{n+1} - t_n - \frac{\Delta\tau}{2}(u_n^3 + u_{n+1}^3) = 0. \tag{5.6}$$

The discretisation (5.5),(5.6) admits the discrete self-similar solution

$$u_n = \hat{U} z^{n/3}, \quad t = z^n.$$

On substituting into (5.5),(5.6) and solving the resulting algebraic equation we then have

$$z^{1/3} = \frac{(1 + \Delta\tau/2)}{(1 - \Delta\tau/2)} = e^{\Delta\tau} + \mathcal{O}(\Delta\tau^3) \tag{5.7}$$

and

$$\hat{U}^3 = \frac{2}{\Delta\tau}\frac{(z-1)}{(z+1)} = 3 + \mathcal{O}(\Delta\tau^2). \tag{5.8}$$

Observe that both of these results are consistent with the error estimates given by Theorem 3.3.

Taking $\Delta\tau = 0.2$ we find that

$$z^{1/3} = 1.2222222.., \quad \hat{U}^3 = 2.922330097...$$

Now consider a general solution of (5.1). For example at $t = 1$ we set $u = 1$ for both the continuous and the discrete problems. The solution of the continuous problem is then given by

$$u = (3t - 2)^{1/3} \tag{5.9}$$

so that

$$t^{-1/3}u \to 3^{1/3} \quad \text{as} \quad t \to \infty.$$

In Figure 5.1 we plot t_n and u_n^3 as functions of τ for the case of $\Delta\tau = 0.2$.

In Figure 5.2 we plot u_n^3/t_n as a function of τ in this case. It is clear from this plot that the value of u_n^3/t_n is asymptotic to 2.922330097 in the limit of $\tau \to \infty$.

Finally in Figure 5.3 we plot the value of $u(t_n)/u_n - 1$ as a function of τ. Here we see that as predicted from Corrollary 3.5 this error is asymptotically constant in the limit of large τ and converges to the final value 0.0087055 which is proportional to $\Delta\tau^2$.

Example 2 A-posteriori scaling.

We now consider the same example as above, but this time introduce a scaling a-posteriori, in a manner more closely related to the use of an adaptive method.

Consider the original problem

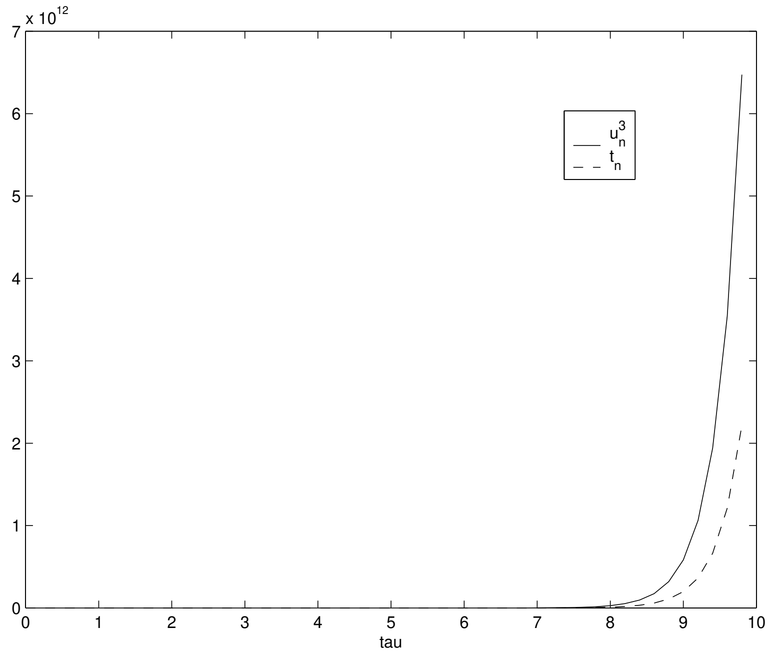

Figure 5.1: t_n and u_n^3 as functions of τ for the case of $\Delta\tau = 0.2$, in example 1.

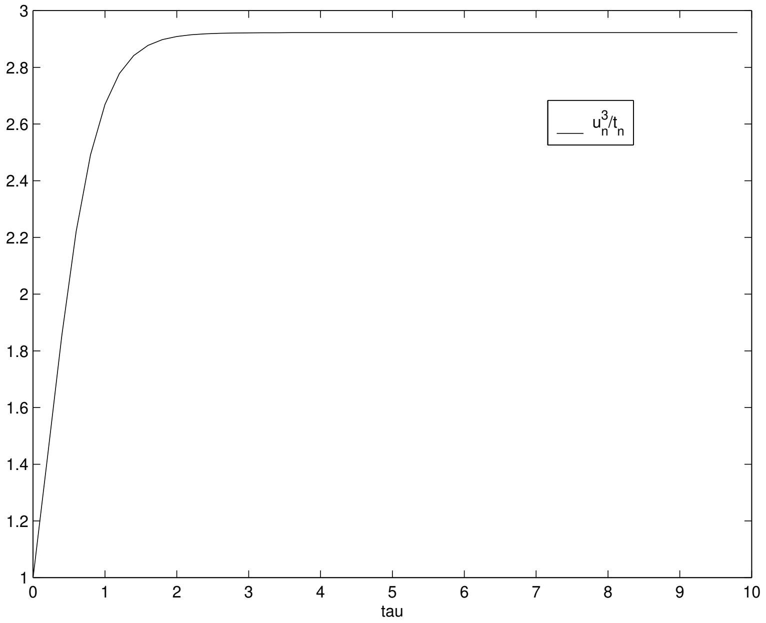

Figure 5.2: u_n^3/t_n as a function of τ, in example 1.

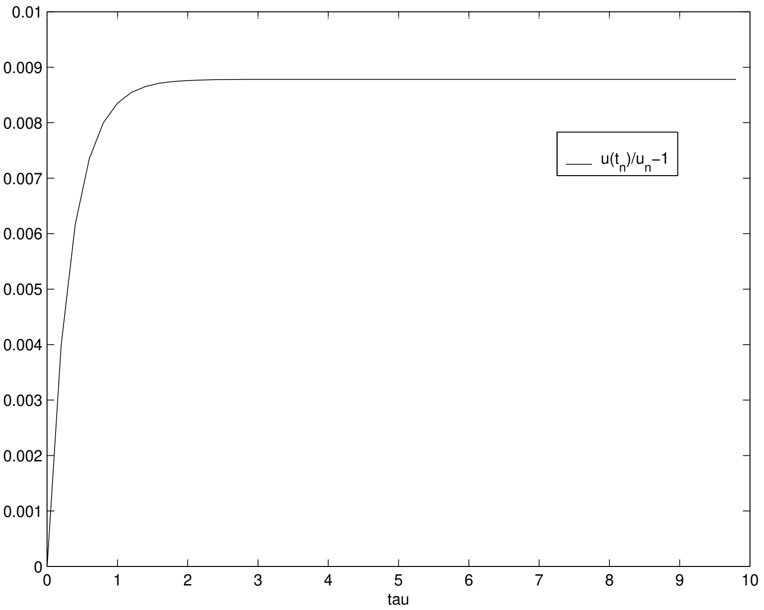

Figure 5.3: $u(t_n)/u_n - 1$ as a function of τ, in example 1.

$$\frac{du}{dt} = u^{-2} \tag{5.10}$$

and approximate u at time t_n by u_n, where the time difference $\Delta t_n = t_{n+1} - t_n$ will be determined during the calculation. Using a trapezoidal discretisation we have

$$u_{n+1} - u_n = \frac{\Delta t_n}{2} \left(\frac{1}{u_n^2} + \frac{1}{u_{n+1}^2} \right). \tag{5.11}$$

Now the local truncation error of the trapezoidal rule is estimated as $e = C(\Delta t_n)^3 u^{(3)}$ for appropriate constant C. Differentiating the differential equation (5.10) twice we have

$$u^{(3)} = \frac{10}{u^8},$$

so that the relative local truncation error (ignoring the effect of constants) is given by

$$E = \frac{(\Delta t_n)^3}{u^9}.$$

If we evaluate this at u_n and set it equal to $(\Delta\tau)^3$ we then have that

$$\Delta t_n = \Delta\tau u_n^3.$$

Substituting this into our scheme gives the adaptively rescaled scheme

$$u_{n+1} - u_n = \frac{\Delta\tau}{2} u_n^3 \left(\frac{1}{u_n^2} + \frac{1}{u_{n+1}^2} \right) \tag{5.12}$$

together with

$$t_{n+1} - t_n = \Delta\tau u_n^3. \tag{5.13}$$

As before the system (5.12),(5.13) admits a discrete self-similar solution of the form

$$u_n = \hat{U} z^{n/3}, \quad t_n = z^n$$

for which z and $\hat{U}$ satisfy the algebraic equations

$$z^{1/3} - 1 = \frac{\Delta\tau}{2}\left(1 + \frac{1}{z^{2/3}}\right), \tag{5.14}$$

and

$$z - 1 = \Delta\tau \hat{U}^3. \tag{5.15}$$

For small $\Delta\tau$ this has the solution

$$z^{1/3} = 1 + \Delta\tau - \Delta\tau^2 + \mathcal{O}\left(\Delta\tau^3\right), \quad \hat{U}^3 = 3 - 5\Delta\tau^2 + \mathcal{O}\left(\Delta\tau^3\right).$$

It is interesting that in this example the calculated value of $\hat{U}^3$ is correct to $\mathcal{O}\left(\Delta\tau^2\right)$ even though the discretisation of the differential equation given by (5.12),(5.13) is of a lower order of accuracy. It is not completely clear why this has occured for this example and is presumably due to the action of higher symmetries. We conclude from this example that, as predicted in section 4, the use of a careful adaptive method gives similar results to the use of a rescaling (as in example 1) based upon group invariance.

Example 3 Gravitational collapse.

Consider the one-dimensional gravitational problem

$$\frac{dr}{dt} = v, \quad \frac{dv}{dt} = -r^{-2}. \tag{5.16}$$

This has the scaling invariance

$$t \to \lambda t, \quad r \to \lambda^{2/3} r, \quad v \to \lambda^{-1/3} v$$

and constant energy

$$E = \frac{v^2}{2} - \frac{1}{r}. \tag{5.17}$$

(The system is also invariant under reflexions and translations in time.)

There are two distinct self-similar solutions with zero energy given by

(a) the *expanding* solution

$$r = Rt^{2/3}, \quad v = Vt^{-1/3} \tag{5.18}$$

and

(b) the *collapsing* solution

$$r = R(T-t)^{2/3}, \quad v = -V(T-t)^{-1/3} \tag{5.19}$$

where T is an arbitrary finite (collapse) time. Here in both cases we have

$$R^3 = \frac{9}{2}, \quad V = \frac{2}{3}\left(\frac{9}{2}\right)^{1/3}. \tag{5.20}$$

The latter solution is of most interest to us as it forms a singularity in a finite time in which $r \to 0$ and $v \to -\infty$. We immediately observe that it is difficult to capture such behaviour if a fixed time-step is used. Indeed, an explicit method will always give a bounded solution, and an implicit method may not have soluble algebraic equations.

If we set $g = r^{3/2}$ then we obtain an invariant system given by

$$\frac{dr}{d\tau} = r^{3/2} v, \quad \frac{dv}{d\tau} = -r^{-1/2}, \quad \frac{dt}{d\tau} = r^{3/2}. \tag{5.21}$$

For this system a collapsing self-similar solution can be given by

$$r = Re^{2\lambda\tau/3}, \quad v = -Ve^{-\lambda\tau/3}, \quad t = T - e^{\lambda\tau} \tag{5.22}$$

where

$$\lambda = -\left(\frac{9}{2}\right)^{1/2}.$$

Observe that as $\tau \to \infty$ we have $t \to T$ and that $t = T - 1$ at $\tau = 0$.

Now consider solving (5.21) by using the trapezoidal rule with step-size $\Delta\tau$. In this case the scheme admits a discrete collapsing self-similar solution given by

$$r_n = \hat{R} z^{2n/3}, \quad v_n = -\hat{V} z^{-n/3}, \quad t_n = T_{\Delta\tau} - z^n.$$

Here $T_{\Delta\tau}$ is a discrete collapse time which need not necessarily coiincide with the true collapse time T. The constants $\hat{R}, \hat{V}$ and $z < 1$ then satisfy the algebraic equations

$$\hat{R}(z^{2/3} - 1) + \frac{\Delta\tau}{2} \hat{R}^{3/2} \hat{V}(z^{2/3} + 1) = 0, \tag{5.23}$$

$$\hat{V}(z^{-1/3} - 1) - \frac{\Delta\tau}{2} \hat{R}^{-1/2}(z^{-1/3} + 1) = 0, \tag{5.24}$$

$$-(z - 1) - \frac{\Delta\tau}{2} \hat{R}^{3/2}(z + 1) = 0, \tag{5.25}$$

Recall that following the predictions of Theorem 3.3 we have

$$\hat{R} = R(1 + \mathcal{O}(\Delta\tau^2)), \quad \hat{V} = V(1 + \mathcal{O}(\Delta\tau^2)), \quad z = e^{\lambda\Delta\tau}(1 + \mathcal{O}(\Delta\tau^3))$$

where, giving their numerical values, we have:

$$R = 1.65096, \quad V = 1.100642.$$

The resulting values are as given below:

$\Delta\tau$	$\hat{R}$	$\hat{V}$	z
0.2	1.63913	1.10184	0.65309
0.1	1.64798	1.10094	0.80867
0.05	1.65021	1.10071	0.89931

The results in this table are fully consistent with the given error estimates.

Similarly we may also use a forward Euler discretisation of the same system. This gives a very similar discrete self-similar collapse solution for which the corresponding values are given by:

$\Delta\tau$	$\hat{R}$	$\hat{V}$	z
0.2	1.46704	1.04761	0.64461
0.1	1.55633	1.07440	0.80584
0.05	1.60298	1.08760	0.89852

As expected these values converge more slowly to the true values, exhibiting a first order rate of convergence.

Now consider a numerical implementation of the forward Euler method, for this problem. For initial values we take $r = 1$ and $v = 0$ at $t = 1$. This problem then has the exact solution given by the quadrature

$$t = 1 + \int_r^1 \frac{\sqrt{s}}{\sqrt{2(1-s)}} ds, \tag{5.26}$$

with a gravitational collapse occuring when

$$T = 1 + \frac{\pi}{2\sqrt{2}} = 2.110720735.$$

The true solution for these values is not self-similar (indeed it has energy $E = 1$) but it converges toward a true self-similar solution as the collapse time is approached.

Using the rescaled method we firstly calculate the value of the discrete collapse time T_Δ as a function of $\Delta\tau$, where T_Δ is estimated as the first value of t_n at which $r_n < 10^{-6}$. These results are given below:

$\Delta\tau$	$T_{\Delta\tau}$	$T_{\Delta\tau} - T$
0.2	2.2758	0.1651
0.1	2.1925	0.0818
0.01	2.1188	0.0081
0.001	2.1115	0.0008

These results give convincing evidence that for this method

$$T_{\Delta\tau} \approx T + 0.8\Delta\tau$$

thus exhibiting first order convergence to the true collapse time, consistent with the rate of convergence of the forward Euler scheme.

Now consider behaviour close to collapse keeping $\Delta\tau$ fixed at $\Delta\tau = 0.2$.

In Figure 5.4 we plot t_n and r_n both as functions of τ. Observe that t_n tends towards the constant value of T_Δ whilst r_n tends to zero. In Figure 5.5 we present a plot or r_n as a function of t_n in this case. Observe the singular nature of collapse of the solution. Now, using the collapse time given above we may rescale the solution by calculating $s_n = r_n(T_{\Delta\tau} - t_n)^{-2/3}$ and $w_n = v_n(T_{\Delta\tau} - t_n)^{1/3}$.

These quantities are plotted in Figure 5.6 as functions of n. Observe that both s_n and w_n converge as n increases to the respective constants $\hat{R} = 1.467042$ and $\hat{V} = 1.104761$ identified in the earlier analysis.

Thus the discrete solution also converges to the discrete self similar solution when rescaled with the correct discrete collapse time.

For completeness we now consider the energy of the discrete self-similar solution. If we initially define a discrete energy by

$$E_n = \frac{1}{2}v_n^2 - \frac{1}{r_n},$$

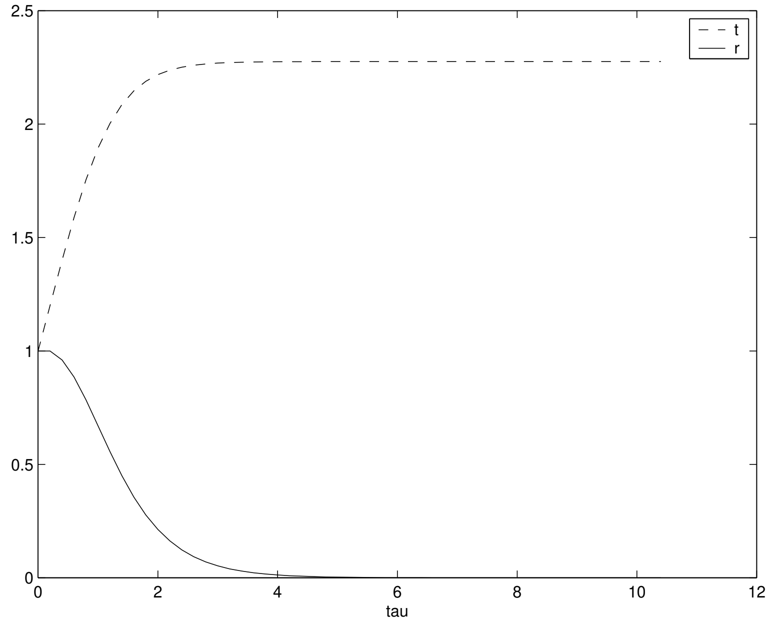

Figure 5.4: Convergence properties of t_n and r_n as functions of τ, in example 3.

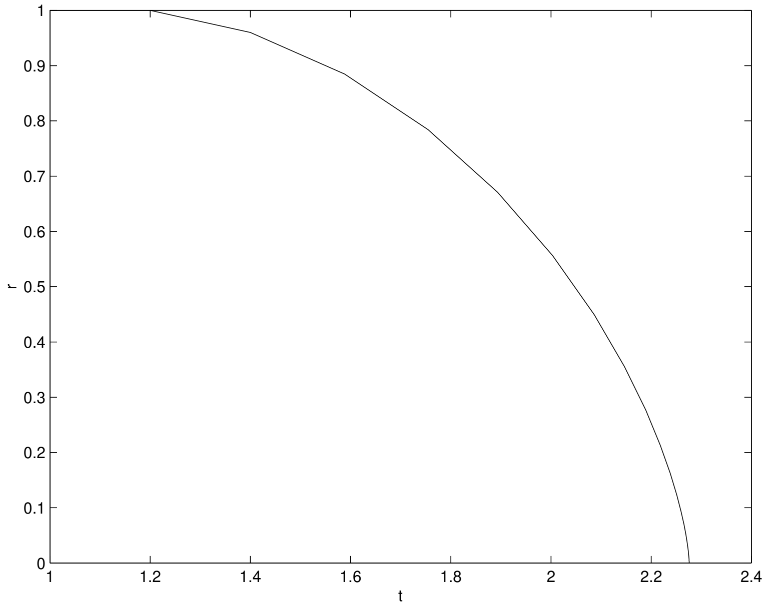

Figure 5.5: The collapse of r as $t \to T$, in example 3.

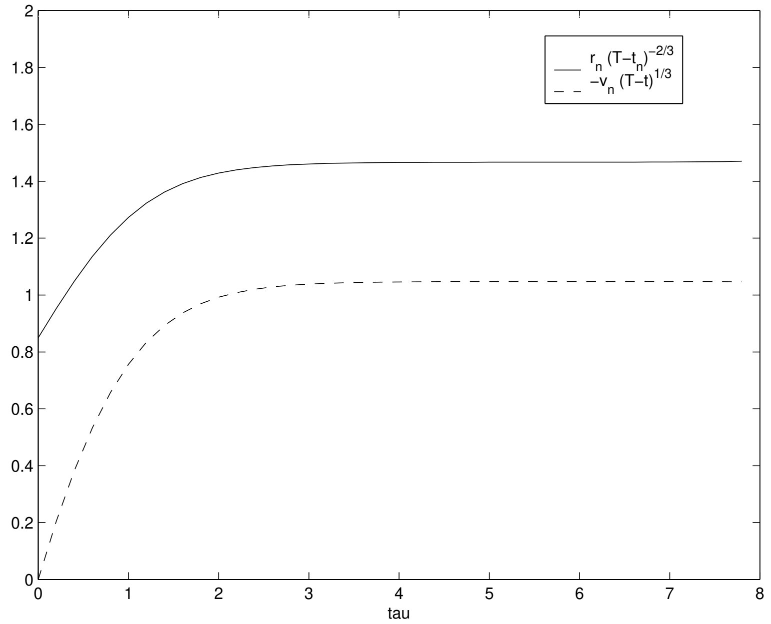

Figure 5.6: Convergence of scaled solutions, in example 3.

then for the discrete self-similar solution

$$E_n = z^{-2n/3}\left(\frac{1}{2}\hat{V}^2 - \frac{1}{\hat{R}}\right) = z^{-2n/3}\hat{E}.$$

For a method in which

$$\hat{R} = R(1 + \mathcal{O}(\Delta\tau^p)), \quad \hat{V} = V(1 + \mathcal{O}(\Delta\tau^p))$$

we then have on substitution that

$$E_n = z^{-2n/3}\hat{E}$$

where

$$\hat{E} = \mathcal{O}(\Delta\tau^p)$$

so that E_n grows without bound as $n \to \infty$. Values of $\hat{E}$ for the forward Euler discretisation are as given below:

$\Delta\tau$	$\hat{E}$
0.2	-0.132898
0.1	-0.065366
0.05	-0.0324047

The divergence of the energy does not on first sight, appear to be very satisfactory, however, we note that the correct dynamics of the solution is recovered even though E_n is not constant.

Part of the difficulty here is that we are not really using the best definition for the discrete energy. Suppose instead that we define a discrete energy by

$$E_n = \frac{1}{2}\left(\frac{V}{\hat{V}}\right)^2 v_n^2 - \left(\frac{\hat{R}}{R}\right)\frac{1}{r}$$

then the coefficients in the redefined energy differ from those in the original definition by the small contribution $\mathcal{O}(\Delta\tau^p)$ and the redefined discrete energy of the self-similar solution is zero.

6 Conclusions

We have shown in this paper that scaling invariance has the unique property amongst general transformations, that the properties of discretisation and invariance commute. Perhaps the most significant feature of this property is that the resulting numerical solutions accurately reproduce (even singular) self-similar solutions for arbitrary large times with a discretisation error that does not grow with time. This feature occurs both with a-priori and (suitably chosen) a-posteriori scaling strategies. Significant questions remain. For example, what is the effect of using a rescaling strategy based on succesive halving of the step-size? Furthermore, what is the best adaptive approach in problems (such as Hamiltonian or reversible problems) for which scaling invariance is only part of the underlying geometry of the solution? We leave these as subjects for further research.

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