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Invariant numerical methods

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SUMMARY

The discretization of partial differential equations can produce numerical errors, and in particular symmetry errors. Typically the symmetry is *fitted* into the numerical method based on the relative merits of physically aligning the mesh, solving in the natural coordinate frame or modifying the truncation error. In this paper we will consider two alternative approaches developed from *capturing* the underlying symmetries, inherent in the partial differential equations, in the numerical method. The invariant numerical methods are developed from the extension of Lie group theory to discretized equations using discrete invariants and the technique of invariantization for the heat equation. Their performances against more traditional schemes will be presented. © British Crown Copyright 2008/MOD. Reproduced with permission. Published by John Wiley & Sons, Ltd.

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KEY WORDS: invariance; discretization; symmetry; Lie groups; heat equation; invariantization

1. INTRODUCTION

The discretization of partial differential equations can produce inaccuracies, and in particular symmetry errors. Typically the symmetry is *fitted* into the numerical method based on three approaches. The first is to align the mesh with the underlying symmetry and adapt the numerical method accordingly. Examples of this type of approach are given by Caramana and Whalen [1] and Margolin and Shashkov [2]. A second approach is to use the natural coordinate frame and to use a coordinate transformation from physical to computational space. For this type of strategy the particular symmetry is contained within the Jacobian for the transformation and is embedded in the Geometric Conservation Law [3]. Finally, the third technique is to modify the numerical method so that the asymmetries inherent within the truncation terms are reduced or eliminated [4]. Partial differential equations remain unchanged when certain transformations are performed; these

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symmetries leave the equations invariant after a given transformation. However, in general the discretized equations do not preserve these symmetries. There is a clear connection between the symmetries that the computational scientist wishes to preserve and those that leave the partial differential equations invariant. Lie group theory is a general way of determining these symmetries [5] and has been used to find analytic solutions to the radiation hydrodynamics equations [6] and Inertial Confined Fusion [7]. The extension to discretized equations has been considered by many authors, particularly from the *Geometric Integration* community, and it is recommended that the reader consult the review article by Levi and Winternitz [8] for an in depth discussion. In this paper we consider two different type of invariant numerical method[§] for the linear heat equation. The first approach was based on the scheme by Bakirova *et al.* [11] in terms of discrete invariants. One of the main weaknesses of this approach is the problem of how to assemble the invariants into a stable and accurate numerical method. The second approach was based on the invariantization scheme by Kim [12]. This technique stems from the concept of moving frames, developed by Fels and Olver [13], where an existing numerical scheme is invariantized to carry symmetry structures of the partial differential equations. For a given numerical method with known stability and consistency properties, the invariantization process adds invariant properties in a way that is more intuitive than the first approach.

In the paper we first describe the heat equation and the type of solutions we wish to solve for. We next go onto describe the two invariant numerical methods and the traditional schemes we will use. Next we will present some results. At each stage comparisons are made against results from the more traditional schemes. Finally, a number of conclusions are drawn from this work.

2. LINEAR HEAT EQUATION

We consider the linear heat equation with unit viscosity $\partial u/\partial t = \partial^2 u/\partial x^2$, where $u = u(x,t)$ is the dependent variable and x and t are the independent variables. This equation admits six point-wise symmetries and one infinite dimensional symmetry [5], from which it is possible to derive invariant solutions. However, in general these solutions represent a subclass of a wider set of solutions that are non-invariant. In this paper we will consider the performance of the different numerical methods for the Galilean invariant solution $u(x,t) = \exp[-x^2/(4(t+\alpha))]/\sqrt{(t+\alpha)}$, where $u(x \to \pm\infty, t) = 0$, and for the non-invariant solution $u(x,t) = \sin(\pi x)\exp(-t\pi^2) + \alpha$, where $u(x=0,t) = \alpha$ and $u(x=1,t) = \alpha$.

3. NUMERICAL METHODS

Our first approach uses the Bakirova invariant scheme (BIS) based on discrete invariants with invariance built into its heart. It is an explicit scheme for the solution and trajectory of the mesh

[§] As an alternative description these methods will be known as SYNChronized numerical methods [9, 10] (SYmmetries of the partial differential equations are numerically captured).

points coupled to changes to the dependent variable. The scheme takes the form,

$$\Delta x = \frac{2\tau^n}{h_{i+}^n + h_{i-}^n}\left[\frac{h_{i-}^n}{h_{i+}^n}\ln\left(\frac{u_{i+1}^n}{u_i^n}\right) - \frac{h_{i+}^n}{h_{i-}^n}\ln\left(\frac{u_{i-1}^n}{u_i^n}\right)\right]$$

$$u_i^{n+1} = \frac{u_i^n \exp\left(-\frac{1}{4}\frac{(\Delta x)^2}{\tau^n}\right)}{\sqrt{\left[1 - \frac{4\tau^n}{h_{i+}^n + h_{i-}^n}\left[\frac{1}{h_{i+}^n}\ln\left(\frac{u_{i+1}^n}{u_i^n}\right) + \frac{1}{h_{i-}^n}\ln\left(\frac{u_{i-1}^n}{u_i^n}\right)\right]\right]}} \tag{1}$$

where the mesh spacings at the nth time level are given by $h_{i-}^n = x_i^n - x_{i-1}^n$, $h_{i+}^n = x_{i+1}^n - x_i^n$ and the change in node position over the course of a time-step τ^n is given by $\Delta x = x_i^{n+1} - x_i^n$. The mesh stencil used for the scheme is illustrated in Figure 1. In general the method is $O(\tau^n, h_{i+}^n h_{i-}^n)$ accurate (for small mesh distortions) but has some special properties when used with the Galilean invariant solution. We will discuss this further in the next section. Owing to space limitations it is recommended that the reader consult the paper by Bakirova for more information. For this work we also developed a predictor corrector[¶] version of this scheme (pcBIS) to improve its temporal accuracy. Our second approach uses the invariantization of the forward in time centred scheme (IFTCS) based on the work by Kim. It is $O(\tau, h^2)$ accurate and takes the form,

$$u_i^{n+1} = u_i^n \Bigg/ \sqrt{\left[1 + \frac{4\tau}{h^2}\left[\ln\left(\frac{2u_i^n}{u_{i-1}^n + u_{i+1}^n}\right)\right]\right]} \tag{2}$$

Unlike the BIS method the mesh remains fixed. For convenience we also construct a predictor corrector version of this scheme (pcIFTCS) to improve temporal accuracy. We consider two traditional numerical methods. For the first we use the forward in time centred scheme (FTCS) given by,

$$u_i^{n+1} = u_i^n + \tau(u_{i+1}^n + u_{i-1}^n - 2u_i^n)/h^2 \tag{3}$$

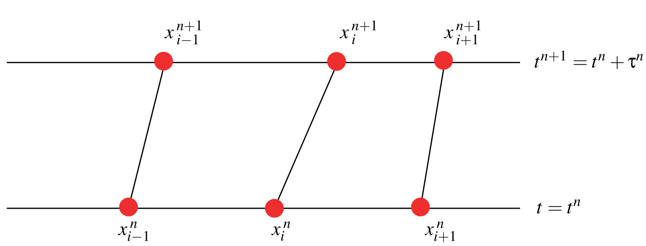

Figure 1. Stencil used in the Bakirova scheme.

[¶]Half time-step predictor followed by full time-step corrector.

As shown by Bakirova this scheme does not preserve Galilean invariant, but like the BIS method it is $O(\tau, h^2)$ accurate. For improved temporal accuracy we use a predictor corrector version of the FTCS method (pcFTCS) with $O(\tau^2, h^2)+O(\tau h^2)$ accuracy.

4. RESULTS

In all presented figures log scales were used. The error is taken to be an average over all spatial points defined by $|\text{Error}|=(1/N)\sum_{i=1}^{N}|u_i^n - u_a(x_i^n, t^n)|$, where $u_a(x_i^n, t^n)$ is the analytic solution.

We first consider the Galilean invariant solution with $\alpha=1$, $x\in[-10,10]$ and $t\in[0,0.1]$. We consider the effect on numerical error of increased number of time-steps Δt within a fixed temporal interval and for fixed spatial resolution Δx. We consider an initial spatial resolution of $\Delta x=0.2$ and initial time-step $\Delta t=\Delta x^2/2$ with results illustrated in Figure 2. It is observed that there is a discontinuity in the error for both the FTCS and IFTCS methods. This occurs when the time-step drops to the point when it is a third of its initial value, and corresponds to a reduction of spatial error from $O(h^2)$ to $O(h^4)$. For this test the best scheme is the BIS method because it can be shown that the scheme has machine order accuracy for the invariant solution. However, it is observed that the error is slowly increasing (due to roundoff error) but remains significantly better than the other methods. It is also noted that the invariance properties of the BIS method are lost when the pcBIS method was used. However, the pcBIS has better than first-order temporal accuracy because the error continues to decrease with increased number of time-steps. For all other schemes the errors begin to converge to some constant value, revealing the first-order temporal accuracy of the schemes. From this test it is noted that the highest errors are from the IFTCS and pcIFTCS methods. The invariantization process has had a negative effect on the FTCS and pcFTCS approaches. We now consider the overall convergence rate for all schemes by fixing the time-step control to be $\Delta t=\Delta x^2/2$ (upper bound used in FTCS) with the results illustrated in Figure 3. The BIS is the best overall scheme in terms of error but it slowly increases with finer resolution. All other schemes are second-order accurate and converging. It is observed that the errors for the FTCS, IFTCS and pcBIS methods are very close to one another, and that the errors

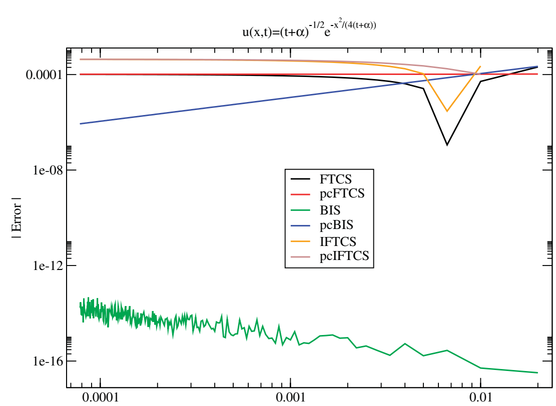

Figure 2. Effect of increased number of smaller time-steps on numerical error for invariant solution.

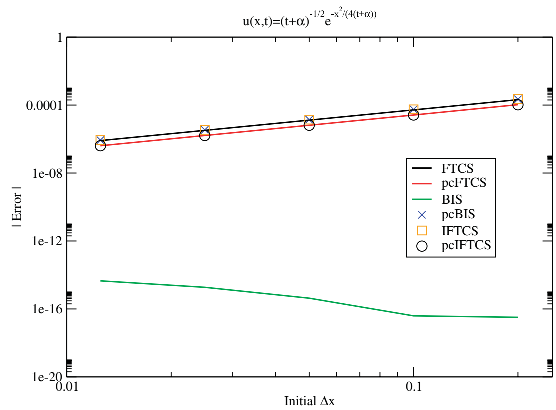

Figure 3. Overall convergence rate for invariant solution.

Table I. Relative computational cost for the different schemes.

Equation	N	Time	FTCS	pcFTCS	BIS	pcBIS	IFTCS	pcIFTCS
$(t+\alpha)^{-1/2}\exp(-x^2/(4(t+\alpha)))$	400	1.0	1.0	1.86	19.1	36.4	10.5	19.4
$\sin(\pi x)\exp(-t\pi^2)+\alpha$	400	0.1	1.0	1.68	22.9	48.5	5.1	9.8

for the pcFTCS and pcIFTCS methods are also very close to one another. It is observed that the latter has lower overall error than the former. It is clear that the invariantization process has had a neutral affect on the FTCS and pcFTCS approaches. In terms of relative computational cost, presented in Table I, the BIS method offers the best accuracy, but at a higher cost, with respect to the FTCS method. The invariantization schemes do not offer significant improvements in accuracy for a given cost with respect to the traditional methods.

We now consider the non-invariant solution with $x\in[0,1]$ and $t\in[0,1.0]$. It is observed that for the BIS and pcBIS methods, $u(x,t)$ must be greater than zero. This imposes a severe restriction on their overall applicability. There are less issues with the invariantization schemes provided it is restricted to one point, such as at the boundary. For convenience we set $\alpha=16/\pi$ to guarantee $u(x,t)>0$. As before we consider the effect of time-stepping Δt for a given spatial resolution $\Delta x=0.01$. These results are illustrated in Figure 4. Again it is observed that there is a discontinuity in the error for the FTCS and IFTCS methods, but it is much sharper. It is also observed that the BIS method also suffers from a similar dip at the same point. Overall the methods converge to similar values with the IFTCS performing the best. Therefore, the BIS and pcBIS approaches do not offer any significant benefits with respect to other methods. We now consider the overall convergence rate for all schemes by fixing the time-step control to be $\Delta t=\Delta x^2/2$ with the results illustrated in Figure 5. All schemes are second-order accurate and converging, with the worse being the FTCS method and best the pcFTCS method in terms of overall error. All other methods are in between. Therefore, the traditional pcFTCS method outperforms the invariant methods in terms of accuracy and cost.

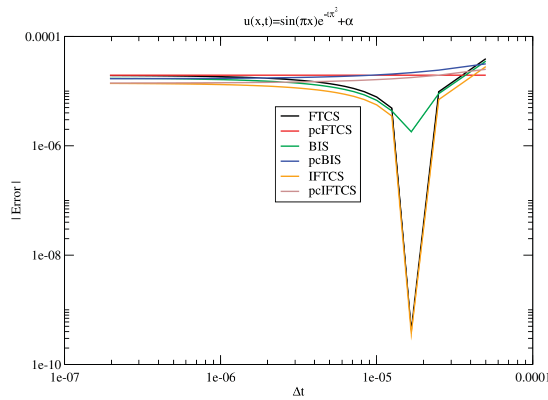

Figure 4. Effect of increased number of smaller time-steps on numerical error for non-invariant solution.

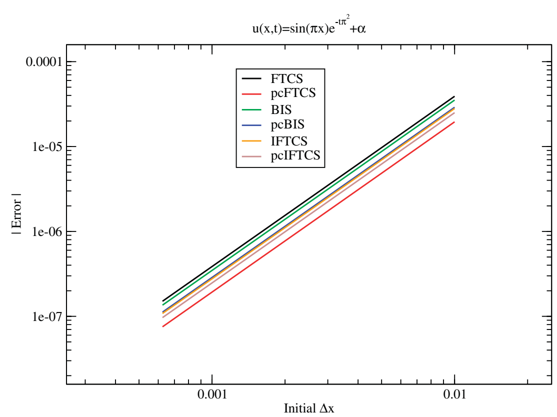

Figure 5. Overall convergence rate for non-invariant solution.

5. CONCLUSIONS

In this paper we have presented results for two different invariant numerical methods and compared them against two traditional numerical methods. For the invariant solution considered the BIS method outperforms all other methods in terms of numerical accuracy. For this problem the invariantization schemes do not offer any significant improvements in accuracy for a given cost with respect to the traditional methods. For the non-invariant solution, the traditional pcFTCS method outperforms the invariant methods in terms of accuracy and cost. For this type of problem, the BIS and pcBIS were found to be ill defined for regions where $u(x,t)=0$. This presents a severe restriction on their overall applicability. For the invariantization schemes provided $u(x,t)=0$ is restricted to the boundaries this will not effect their applicability.

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