

SYNChronised numerical methods

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Abstract

The discretization of partial differential equations will produce inaccuracies, and in particular symmetry errors. Traditionally, symmetry is *fitted* into the numerical method[7] based on three approaches. The first is to align the mesh with the underlying symmetry and adapt the numerical method accordingly[4, 14]. 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 a Geometric Conservation Law[17]. Finally, a third approach is to modify the numerical method to reduce the asymmetric errors, inherent within the truncation terms, by using more information from the wider computational mesh stencil[13]. Partial differential equations remain unchanged when certain transformations are performed; these *symmetries* leave the equations invariant after a given transformation. Lie group theory has been shown to be a general way of determining these symmetries[15, 3, 16, 12] and has been used to find analytic solutions to many partial differential equations, and in particular, hydrodynamic related equations[5, 2]. However, in general the discretized equations do not preserve these symmetries. By extending Lie groups to the discrete system[8, 9, 6, 10, 11] we will develop guiding principles for SYNChronised numerical methods where the SYmmetries of the partial differential equations are Numerically Captured. By using this framework we will show, through the concept of numerical symmetry breaking, why some numerical techniques are more suitable than others for a given application. ©British Crown Copyright MOD/2013

1. Fundamentals

Lie group theory is the marriage between co-ordinate geometry and group theory. Transformations form a group and are continuous based upon the variation of a group parameter. Lie group theory is based upon transformations of both the independent and dependent variables. For m independent variables $(x_1, \dots, x_m)$ and n dependent variables $(u_1, \dots, u_n)$ these define a $m + n$ dimensional phase space in which all points are treated as independent. They are transformed in a continuous manner based on the group parameter λ and the arbitrarily defined *pointwise* functions thus,

$$\tilde{x}_k = F_k(x_1, \dots, x_m, u_1, \dots, u_n; \lambda) , \quad \tilde{u}_j = F_j(x_1, \dots, x_m, u_1, \dots, u_n; \lambda) , \quad (1.1)$$

for $1 \leq k \leq m$ and $m + 1 \leq j \leq m + n$ and where the tilde represents the transformed variable. It is assumed that all of the functions are continuous and continuously differentiable (C^∞) in all of the variables and λ . Note, there is an identity value $\lambda = \lambda_o$ that leaves the co-ordinates unchanged. Whence,

$$x_k = F_k(x_1, \dots, x_m, u_1, \dots, u_n; \lambda_o) , \quad u_j = F_j(x_1, \dots, x_m, u_1, \dots, u_n; \lambda_o) . \quad (1.2)$$

If we consider an infinitesimal transformations from $\lambda_o \rightarrow \lambda_o + \Delta\lambda$ then they can be written as,

$$\tilde{x}_k = x_k + \xi_k(x_1, \dots, u_1, \dots) \Delta\lambda + O(\Delta\lambda^2), \quad \tilde{u}_j = u_j + \eta_j(x_1, \dots, u_1, \dots) \Delta\lambda + O(\Delta\lambda^2), \quad (1.3)$$

where ξ_k and η_j are respectively the *infinitesimal generators* for the k -th independent and j -th dependent variables. The generator for the group can now be written,

$$\mathcal{X} = \xi_1 \frac{\partial}{\partial x_1} + \dots + \xi_m \frac{\partial}{\partial x_m} + \eta_1 \frac{\partial}{\partial u_1} + \dots + \eta_n \frac{\partial}{\partial u_n}. \quad (1.4)$$

The computational scientist will be familiar with the use of transformations mapping from physical to computational space[17]. However, for these types of transformations they are geometric in nature. Furthermore, they assume that both the time t and dependent variables $(u_1, \dots, u_n)$ remain unchanged after the transformation. When compared to the transformations Eq.(1.1) they represent a subset of the Lie group transformations. For the general partial differential equation,

$$G(x_k, u_i, u_{i,m}, u_{i,mn}, \dots) = 0, \text{ where } u_{i,m} = \frac{\partial u_i}{\partial x_m}, \quad u_{i,mn} = \frac{\partial^2 u_i}{\partial x_m \partial x_n}, \dots \quad (1.5)$$

the transformed PDE is related to the original PDE by the transformation thus,

$$\tilde{G}(\tilde{x}_k, \tilde{u}_i, \tilde{u}_{i,\tilde{m}}, \tilde{u}_{i,\tilde{m}\tilde{n}}, \dots; \lambda) = G(x_k, u_i, u_{i,m}, u_{i,mn}, \dots; \lambda_o) + \Delta\lambda(\mathcal{X}G) + O(\Delta\lambda^2), \quad (1.6)$$

where λ_o is the identify value that leaves the PDE unchanged, the tilde symbol represents the transformed PDE and the generator $\mathcal{X}$ has been prolonged[15] to include transformations of the partial derivatives found within $G(\dots) = 0$; see next section. For invariance of the PDE $\mathcal{X}G(\dots) = \mathcal{H}(\dots)G(\dots)$ for the arbitrary function $\mathcal{H}(\dots)$ provided $G(\dots) = 0$. Whence,

$$\tilde{G}(\tilde{x}_k, \tilde{u}_i, \tilde{u}_{i,\tilde{m}}, \tilde{u}_{i,\tilde{m}\tilde{n}}, \dots; \lambda) = G(x_k, u_i, u_{i,m}, u_{i,mn}, \dots; \lambda_o). \quad (1.7)$$

2. Extension to Numerical Methods

For a given numerical method (NM) expressed as,

$$G_{\text{NM}}(x_i^n, t_i^n, \tau^n, h_{i+}^n, h_{i-}^n, u_{i-1}^n, u_i^n, u_{i+1}^n, u_i^{n+1}, \dots) = 0, \quad (2.1)$$

it can be written after the Lie group transformation as,

$$\tilde{G}_{\text{NM}}(\dots; \lambda) = G_{\text{NM}}(\dots; \lambda_o) + (\mathcal{X}_{\text{NM}} G_{\text{NM}}) \Delta\lambda + O(\Delta\lambda^2), \quad (2.2)$$

where $\mathcal{X}_{\text{NM}}$ is the group operator which has been prolonged to include the transformations of the numerical method. This operator must now include terms that represent the discrete dependent variables and independent quantities (mesh positions) with respect to λ . For example, Figure 1 illustrates one way that the points (x_i^n, t_i^n, u_i^n) can vary after a transformation. The group operator $\mathcal{X}_{\text{NM}}$ will leave the PDE invariant and for numerical invariance,

$$\mathcal{X}_{\text{NM}} G_{\text{NM}}(\dots) = \mathcal{H}_{\text{NM}}(\dots) G_{\text{NM}}(\dots), \quad (2.3)$$

for the arbitrary discrete function $\mathcal{H}_{\text{NM}}(x_i^n, t_i^n, \tau^n, h_{i+}^n, h_{i-}^n, u_{i-1}^n, u_i^n, u_{i+1}^n, u_i^{n+1}, \dots)$ since $G_{\text{NM}}(\dots) = 0$. Whence,

$$\tilde{G}_{\text{NM}}(\dots; \lambda) = G_{\text{NM}}(\dots; \lambda_o). \quad (2.4)$$

When this is satisfied the numerical method will be SYNChronised with the PDEs. Alternatively, a numerical method satisfying this will be known as a SYNC scheme; SYmmetries of the partial differential equations are Numerically Captured.

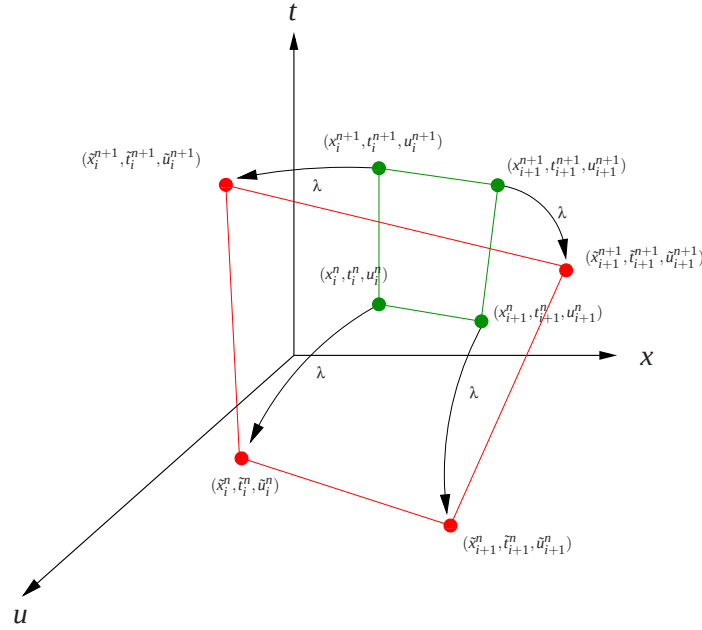


FIGURE 1. Relationship between discrete Lie co-ordinate points.

3. Invariant Truncation Error

Using Taylor's theorem a numerical method can be shown to be equal to a modified equation (ME) in which the original homogeneous PDE now equals a truncation error (TE) source term thus,

$$G_{\text{ME}}(\cdots) = G(\cdots) = \text{TE}(\cdots) . \quad (3.1)$$

By applying the prolonged group operator to the modified equation it will be invariant, like the PDE, when the truncation error is also invariant thus,

$$\chi_{\text{NM}} G_{\text{ME}} = \frac{\delta(\text{TE})}{\delta \lambda} = 0 . \quad (3.2)$$

This is the condition for a SYNChronised numerical method.

4. Numerical Symmetry Breaking

The equations of hydrodynamics can be written in conservation law form as,

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0 , \quad (4.1)$$

where the dependent variable u represents some conserved quantity, such as mass. This equation can be written numerically in explicit Eulerian conservation law form using a fixed mesh (please refer to the books by Hirsch[1] for general descriptions of types of numerical methods) as,

$$G_{\text{NM}}(\cdots; \lambda_o) = u_i^{n+1} - u_i^n + \frac{\tau^n}{h} (F(u_{i-p}^n, \dots, u_{i+q}^n; h, \tau^n) - F(u_{i-1-p}^n, \dots, u_{i-1+q}^n; h, \tau^n)) = 0 , \quad (4.2)$$

where h is the grid spacing (assumed fixed and uniform), τ^n the time-step, and $F(\dots)$ are the numerical flux functions. For simplicity we shall use the notation $F_{i+1/2}^n = F(u_{i-p}^n, \dots, u_{i+q}^n; h, \tau^n)$. The integers p and q define the size of the mesh stencil $p + q + 1$ for the flux functions. The condition that this will be a SYNC scheme is $\mathcal{X}_{\text{NM}} G_{\text{NM}} = \mathcal{H}_{\text{NM}} G_{\text{NM}}$. That is,

$$\frac{\delta u_i^{n+1}}{\delta \lambda} - \frac{\delta u_i^n}{\delta \lambda} + \left(\frac{1}{h} \frac{\delta \tau^n}{\delta \lambda} - \frac{\tau^n}{h^2} \frac{\delta h}{\delta \lambda} \right) (F_{i+1/2}^n - F_{i-1/2}^n) + \frac{\tau^n}{h} \left(\frac{\delta F_{i+1/2}^n}{\delta \lambda} - \frac{\delta F_{i-1/2}^n}{\delta \lambda} \right) = \mathcal{H}_{\text{NM}} G_{\text{NM}} , \quad (4.3)$$

We consider this framework for the non-linear viscous Burgers' equation,

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} , \quad (4.4)$$

where ν is a parameter representing viscosity. The group structure for this equation is given by Hydon, and consists of five groups representing scale invariance, projective invariance, Galilean invariance, temporal and spatial translation. Without loss of generality we shall consider a three point stencil ($p = 0$ and $q = 1$) and by prolonging the five group operators yields,

$$\begin{aligned} \mathcal{X}_{\text{NM}}^1 &= x_i^n \frac{\partial}{\partial x_i^n} + 2t^n \frac{\partial}{\partial t^n} - u_i^n \frac{\partial}{\partial u_i^n} + h \frac{\partial}{\partial h} + 2\tau^n \frac{\partial}{\partial \tau^n} - u_{i-1}^n \frac{\partial}{\partial u_{i-1}^n} - u_{i+1}^n \frac{\partial}{\partial u_{i+1}^n} - u_i^{n+1} \frac{\partial}{\partial u_i^{n+1}} \\ \mathcal{X}_{\text{NM}}^2 &= x_i^n t^n \frac{\partial}{\partial x_i^n} + (t^n)^2 \frac{\partial}{\partial t^n} + (x_i^n - u_i^n t^n) \frac{\partial}{\partial u_i^n} + h t^n \frac{\partial}{\partial h} + (t^n + t^{n+1}) \tau^n \frac{\partial}{\partial \tau^n} + \dots \\ \mathcal{X}_{\text{NM}}^3 &= t^n \frac{\partial}{\partial x_i^n} + \frac{\partial}{\partial u_i^n} + \frac{\partial}{\partial u_{i-1}^n} + \frac{\partial}{\partial u_{i+1}^n} + [1 - \tau^n S_t^+(u_x)] \frac{\partial}{\partial u_i^{n+1}} \\ \mathcal{X}_{\text{NM}}^4 &= \frac{\partial}{\partial t^n} \\ \mathcal{X}_{\text{NM}}^5 &= \frac{\partial}{\partial x_i^n} \end{aligned} \quad (4.5)$$

where S_t^+ is a shift operator. We do not provide the whole structure for $\mathcal{X}_{\text{NM}}^2$ due to its complexity. From $\mathcal{X}_{\text{NM}}^4 G_{\text{NM}}$ and $\mathcal{X}_{\text{NM}}^5 G_{\text{NM}}$ it is immediately obvious that $\mathcal{H}_{\text{NM}} = 0$ and that G_{NM} cannot be a function of x_i^n and t^n . For $\mathcal{X}_{\text{NM}}^1 G_{\text{NM}}$ it can be shown (using the method of characteristics) that the flux can be written in terms of discrete invariants,

$$J_4 = \mathcal{G}(J_1, J_2, J_3) , \quad (4.6)$$

where $\mathcal{G}$ is an arbitrary flux function with the discrete invariants given by,

$$J_1 = \frac{u_{i+1}^n}{u_i^n} , \quad J_2 = \frac{h^2}{\tau^n} , \quad J_3 = u_i^n h , \quad J_4 = \tau^n F_{i+1/2}^n . \quad (4.7)$$

In practice the values of the discrete invariants will be restricted to satisfy numerical stability and monotonicity. It can be shown that the invariant flux function Eq.(4.6) does not satisfy the Galilean and Projective groups. Therefore, a numerical scheme of the type defined by Eq.(4.2) will break the symmetry inherent in the PDE. The lack of invariance lies in the introduction of gradients within some of the prolonged group operators. The Galilean operator includes the gradient term $[1 - \tau^n S_t^+(u_x)]$ and represents the relative motion between the *fixed* and *moving* frames and is illustrated in Figure 2. At $t = t^n$ both frames are coincident, but after a short period τ^n the Galilean frame has moved relative to the fixed frame. Within the fixed frame $x_i^n = x_i^{n+1}$ and within the moving frame $\tilde{x}_i^n = \tilde{x}_i^{n+1}$, but the relative positions between the different frames changes. The value of $\tilde{u}_i^{n+1}$ moves along a trajectory relative to the fixed frame and its value can be thought of as being interpolated from the values within the fixed frame.

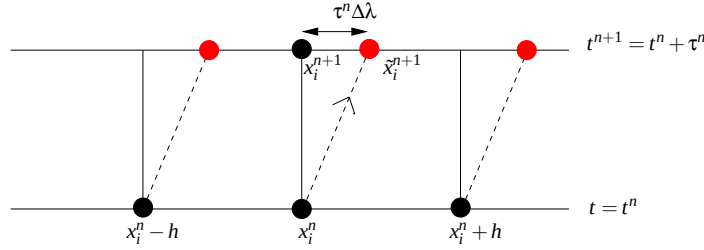


FIGURE 2. Relationship between fixed (black) and moving frames (red).

This is the source of the gradient term. Note, this type of analysis can be applied to the projective operator.

A numerical scheme based upon a fixed stencil can break certain symmetries. A scheme that is SYNChronised with all of the PDEs symmetries is one where the mesh moves to its *natural* positions. In this paper we will not consider how this can be done due to space limitations. However, the reader should consider numerical methods based on discrete invariants[19, 10, 11] and those based on Moving Frames[18, 8].

5. Conclusions

Using Lie group theory we have presented a concise mathematical definition for the invariance of partial differential equations under a given transformation. In this paper this framework was extended to its representative numerical method and it was shown that it can remain invariant only if its truncation error remains invariant. Numerical schemes of this type are SYNChronised with their respective PDEs symmetries. In this paper we have shown how numerical invariance errors are due to numerical symmetry breaking. A scheme that is SYNChronised is one where the mesh moves to its *natural* positions.

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