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A new construction for invariant numerical schemes using moving frames

Une construction nouvelle des schémas invariants utilisant les repères mobiles

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A B S T R A C T

We propose a new approach for moving frame construction that allows to make finite difference scheme invariant. This approach takes into account the order of accuracy and guarantees numerical properties of invariant schemes that overcome those of classical schemes. Benefits obtained with this process are illustrated with the Burgers equation.

R É S U M É

On propose une procédure nouvelle de construction des repères mobiles permettant de rendre invariant les schémas de discrétisation en différences finies. Elle prend en compte l'ordre de consistance et garantit aux schémas invariants de meilleures performances que celles des schémas classiques. On illustre les performances de cette approche sur l'exemple de l'équation de Burgers.

Version française abrégée

Les méthodes numériques construites afin de préserver certaines propriétés liées à la structure géométrique des équations s'appelle les intégrateurs géométriques. Elles permettent de traduire naturellement le comportement qualitatif des solutions ainsi que de réduire les instabilités numériques. En particulier, les schémas invariants permettent de conserver le groupe de symétrie des équations et de réduire les erreurs numériques. Une méthode de construction de tels schémas a été développée par M. Fels et P. J. Olver. Elle est basée sur le concept de repère mobile. Dans cette procédure, la qualité des solutions numériques d'un schéma invariant est entièrement conditionnée par le choix du repère mobile associé au groupe de symétrie. Ce choix est déterminé par le procédé de normalisation d'É. Cartan qui permet de ramener la détermination du répère mobile associé à un groupe continue au choix d'une section transverse de l'orbite d'un élément. Ce procédé possède l'avantage d'exhiber une famille importante de schémas invariant mais ne garantit pas au schéma obtenu des qualités numériques meilleures que le schéma d'origine. Nous proposons une méthode de construction nouvelle des schémas invariants

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utilisant les repères mobiles. Cette méthode peut être décrite sous la forme algorithmique suivante : (i) On considère un schéma discrétisant une EDP et le groupe de symétrie dépendant de paramètres réels de l'EDP, (ii) on transforme le schéma afin d'obtenir un schéma paramétrisé, (iii) on suppose une forme algébrique des paramètres en fonction de coefficients réels, (iv) on calcule les conditions d'équivariance afin que les paramètres de transformation deviennent des repères mobiles, (v) enfin, on calcule les conditions sur les coefficients réels pour que le schéma transformé soit d'un ordre de précision fixé. Ainsi on obtient un schéma invariant dont l'ordre de consistance est déterminé. On illustre les performances de cette approche á travers la construction d'un schéma invariant pour l'équation de Burgers.

1. Introduction

Geometric integrators are numerical methods based on the preservation of equations structure as their conservation laws, their variational properties or their symmetry [1]. They are known to be successful in the reliable reproduction of qualitative behaviours in a solution and also in reducing numerical instabilities. A recent approach to construct invariant numerical schemes using moving frames, as developed by M. Fels and P.J. Olver [2], allows one to preserve symmetry of equations and reduce numerical errors. The method is based on the Cartan's method of normalization: the moving frame is determined from a choice of a cross-section to the group orbit. It has been studied and validated for many classes of differential systems and for partial differential equations (PDE) by P. Kim [3]. But even if this process can perform some very convenient results, its algorithm suffers dramatically of several points: i) the choice of the moving frame (given by the choice of a cross-section) to construct the invariant scheme is unclear: Kim uses some ad hoc pseudo-curvature involved by a knowledge of the solution, ii) chosen moving frames are finally adapted (*adaptive invariantization*) such that the invariance property of the scheme is no more assured, iii) the numerical properties of the invariantized scheme is very sensitive to the choice of the cross-section, iv) the process of invariantization using the normalization method cannot give any guarantee for a good accuracy of the invariant scheme. In this paper, the authors propose an alternate way of constructing invariant numerical schemes that fixes the order of accuracy. The algorithm of construction, described in next sections, is not based on the Cartan's method of normalization.

2. Principle of construction

2.1. Definitions

In this subsection some definitions needed for the construction of invariant numerical schemes are briefly recalled. For more details, we refer the reader to the works of P. Kim [3], P.J. Olver [4,2]. Consider a PDE $F(z) = 0$ over a manifold M. A symmetry of $F(z) = 0$ is a group of transformations G that preserves the set of whole solutions of the equation:

$$F(z) = 0 \Rightarrow F(g \cdot z) = 0 \quad \forall g \in G \tag{1}$$

A numerical application N that stays unchanged under any element of G is said to be G-invariant:

$$N(z) = N(g \cdot z) \quad \forall g \in G \tag{2}$$

For the present purpose, numerical schemes are considered as numerical applications that verify some consistency conditions with the continuous PDE [2]. A numerical scheme is therefore G-invariant if its transformation coincides with itself. Let's now look at particular elements $\rho(z)$ of the group G that depends on the variable z and that verify the equivariance relation:

$$\rho(g \cdot z) = \rho(z) g^{-1} \quad \forall g \in G \tag{3}$$

Such transformations are called moving frames associated to the group G. The fundamental theorem of construction of invariant numerical schemes using moving frames simply states that if a numerical scheme is transformed by a moving frame associated to the group G, then the scheme becomes G-invariant [3]. The new approach proposed in this Note allows one to fix the order of accuracy of the invariant scheme. It can be summarized as follows: start with a classical numerical scheme associated to a PDE whose symmetry group noted G has d finite dimensional 1-parameter subgroups, then (i) express the G-transformed scheme in function of the symmetrization parameters ε_k, for $k = 1, \ldots, d$, (ii) for each ε_k, $k = 1, \ldots, d$, suppose an algebraic form involving the stencil points of the original scheme and some real constant coefficients $\alpha_k^1, \ldots, \alpha_k^\sigma$, where σ is the number of stencil points. (iii) Compute the value of the real constant coefficients such that: a) each ε_k, $k = 1, \ldots, d$, verifies the equivariance property (Eq. 3), and b) the parametrized scheme is at less as accurate than the original scheme. One finally obtains an invariant scheme with a chosen order of accuracy.

Let us compute by this process an invariant explicit numerical scheme for the Burgers' equation. Numerical results are illustrated in the next section.

2.2. Symmetry of the Burgers equation

Consider the Burgers equation for the dependent variable u in a spatial domain Ω for time $t \geqslant 0$:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2} \tag{4}$$

associated with the initial condition $u(x,0) = u_0(x)$, and the condition $u_{|\partial\Omega} = g(t)$ on the boundary $\partial\Omega$ of the domain. The parameter ν is the viscosity. The symmetry group of (4) is composed by the one-parameter transformations [5]: spatial translation: $(x,t,u) \longmapsto (x+\varepsilon_1, t, u)$; time translation: $(x,t,u) \longmapsto (x, t+\varepsilon_2, u)$; projection: $(x,t,u) \longmapsto (\frac{x}{1-\varepsilon_3 t}, \frac{t}{1-\varepsilon_3 t}, (1-\varepsilon_3 t)u + \varepsilon_3 x)$; scale transformation: $(x,t,u) \longmapsto (xe^{\varepsilon_4}, te^{2\varepsilon_4}, ue^{-\varepsilon_4})$; Galilean boost: $(x,t,u) \longmapsto (x+\varepsilon_5 t, t, u+\varepsilon_5)$.

For scheme invariance considerations, the interest is focused on all symmetries except the scale transformation. Indeed, most of numerical schemes are invariant under the space translation, the time translation and the scale transformation. The projection and the Galilean boost are most often broken. Consider the transformation $(x,t,u) \longmapsto (\bar{x}, \bar{t}, \bar{u})$ depending on parameters $\varepsilon_1, \varepsilon_2, \varepsilon_3$ and ε_5:

$$\bar{x} = \frac{(x+\varepsilon_1) + \varepsilon_5(t+\varepsilon_2)}{1-\varepsilon_3(t+\varepsilon_2)}, \qquad \bar{t} = \frac{t+\varepsilon_2}{1-\varepsilon_3(t+\varepsilon_2)}, \qquad \bar{u} = u\big(1-\varepsilon_3(t+\varepsilon_2)\big) + (x+\varepsilon_1)\varepsilon_3 + \varepsilon_5 \tag{5}$$

Let us make invariant under this transformation the method defined by the classical explicit Forward in Time and Centered in Space scheme (FTCS scheme):

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + u_j^n\left(\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}\right) - \nu\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2} = 0 \tag{6}$$

This scheme is computed on a regular and orthogonal mesh such that $\Delta t = t^{n+1} - t^n$ and $\Delta x = x_{j+1} - x_j$. The discretisation stencil is composed by the discrete points $\mathbf{z} = (z_j^{n+1}, z_j^n, z_{j\pm1}^n)$, where $z_j^n = (x_j, t^n, u_j^n)$. For the transformation acting only on the independent variables (the time and the space translations), the same argument as in [3] is used. In order to express the numerical scheme in term of the time step Δt and the spatial step Δx, choose for moving frames:

$$\varepsilon_1 = -x_j, \qquad \varepsilon_2 = -t^n \tag{7}$$

So that we now consider the action of the group G over the stencil points $\mathbf{z}$:

$$z_j^n \mapsto \bar{z}_j^n = \big(0, 0, u_j^n + \varepsilon_5\big) \tag{8}$$

$$z_j^{n+1} \mapsto \bar{z}_j^{n+1} = \left(\frac{\varepsilon_5\Delta t}{1-\varepsilon_3\Delta t}, \frac{\Delta t}{1-\varepsilon_3\Delta t}, u_j^{n+1}(1-\varepsilon_3\Delta t) + \varepsilon_5\right) \tag{9}$$

$$z_{j\pm1}^n \mapsto \bar{z}_{j\pm1}^n = \big(\Delta x, 0, u_{j\pm1}^n + \varepsilon_3\Delta x + \varepsilon_5\big) \tag{10}$$

In order to make ε_3 and ε_5 the moving frames and then to make ρ a moving frame associated to the transformation (8) of G, and to compute the equivariance relation (3), let's choose for their expression a combination of discrete variables which are dimensionally relevant (as $[\varepsilon_3] = [\text{time}]^{-1}$). ε_3 must not have any term in u^{n+1} to keep the explicit form of the numerical scheme. The symmetrization parameter must be at most of degree one to preserve the order of the convective term. Finally the construction of a moving frame from the application ε_3 requires that there are no terms depending on Δx and Δt alone. Similar arguments for ε_5 (of dimension $[\text{length}] \times [\text{time}]^{-1}$) can be built. Suppose then the algebraic form:

$$\varepsilon_3 = \frac{au_{j+1}^n + bu_j^n + cu_{j-1}^n}{\Delta x}, \qquad \varepsilon_5 = du_{j+1}^n + eu_j^n + fu_{j-1}^n \tag{11}$$

where a, b, c and d, e, f are constant real coefficients. Then write down the expression of any transformed stencil points $\bar{\mathbf{z}} = g \cdot \mathbf{z}$ for $g \in G$ by ρ, taking into account the expression of ε_3 and ε_5 given in (11). Substitute then the expression of $\bar{\mathbf{z}}$ following the action (8) of G, the equivariance condition (3) gives the restriction over the coefficients:

$$c - a = 1, \qquad a + b + c = 0, \qquad d - f = 0, \qquad d + e + f = -1 \tag{12}$$

The invariant FTCS (IFTCS) scheme is then:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + u_j^n\left(\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}\right) - \nu\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2} + F = 0 \tag{13}$$

with the constant coefficients (a, b, c, d, e, f) verifying (12) in:

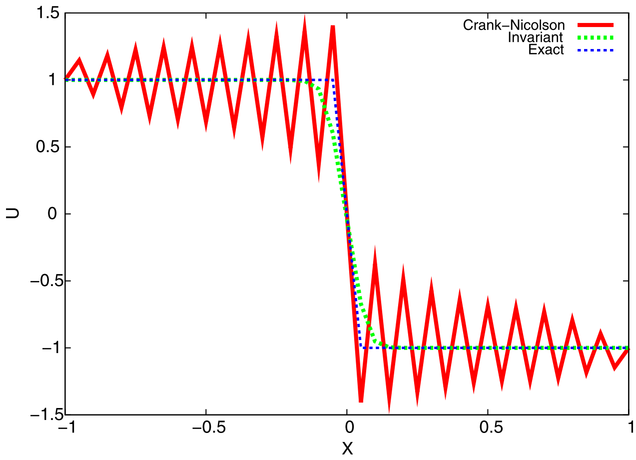


Fig. 1. Burgers equation. Exact solution, implicit Crank–Nicolson scheme, and explicit invariant scheme. Over the spatial domain $\Omega =]-1;1[$ at time $t = 2$. Mesh parameters are set to $\Delta x = \Delta t = 5 \times 10^{-2}$, and the viscosity is $\nu = 75 \times 10^{-5}$.

$$F = -2\left(\frac{au^n_{j+1} + bu^n_j + cu^n_{j-1}}{\Delta x}\right)\left(u^{n+1}_j - u^n_j\right) + \Delta t\left(\frac{au^n_{j+1} + bu^n_j + cu^n_{j-1}}{\Delta x}\right)^2 u^{n+1}_j + \left(du^n_{j+1} + eu^n_j + fu^n_{j-1}\right)\left(\frac{u^n_{j+1} - u^n_{j-1}}{2\Delta x} + \left(\frac{au^n_{j+1} + bu^n_j + cu^n_{j-1}}{\Delta x}\right)\right) \tag{14}$$

The order of accuracy of the IFTCS scheme is obtained by Taylor expansion. The added term is consistent with:

$$F = (a+c)\frac{\Delta x}{2}\frac{\partial^2 u}{\partial x^2}\left(-u - 2\Delta t\frac{\partial u}{\partial t}\right) + \Delta t\left(2\frac{\partial u}{\partial x}\frac{\partial u}{\partial t} + \left(u + \Delta t\frac{\partial u}{\partial t}\right)\left(-\frac{\partial u}{\partial x} + (a+c)\frac{\Delta x}{2}\frac{\partial^2 u}{\partial x^2}\right)^2\right) + O\left(\Delta t, \Delta x^2\right) \tag{15}$$

The condition for the transformed scheme to be of the same order of accuracy as the original classical FTCS scheme is then $a + c = 0$. Therefore ε_3 has an unique expression:

$$\varepsilon_3 = -\frac{u^n_{j+1} - u^n_{j-1}}{2h} \tag{16}$$

The expression of ε_5 is given by (11). The coefficients d, e, f verify the equivariance condition (12).

Remark 1. The cross-section associated to ε_3 is $\bar{u}^n_{j+1} - \bar{u}^n_{j-1} = 0$. In the process of invariantization exposed by P. Kim [3], there exists no arguments to choose this cross-section. Other choices of cross-section would give invariant schemes whose numerical properties would probably not overcome the classical FTCS scheme ones.

3. Numerical results

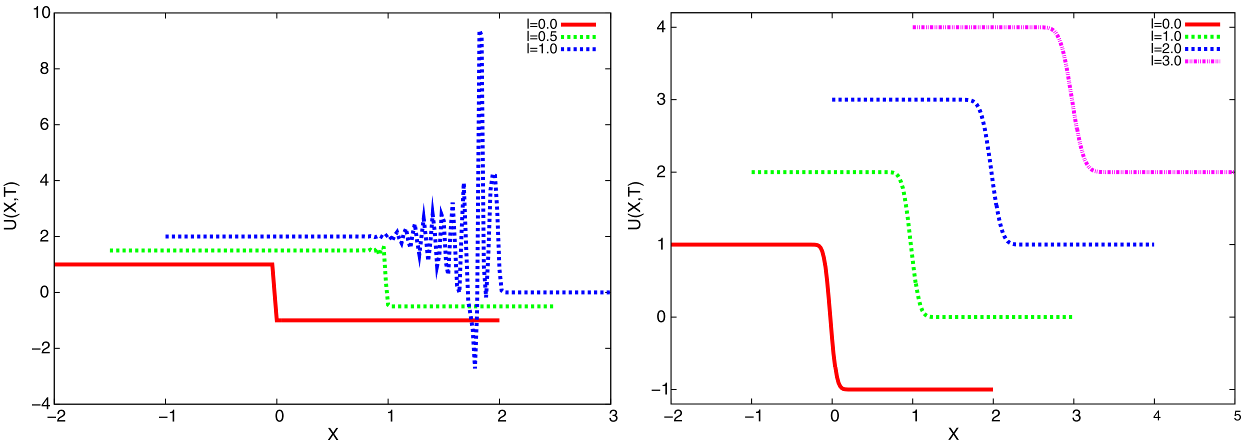
3.1. Pseudo-shock test

Consider the Burgers equation (4) on a bounded domain Ω. The initial and the boundary conditions are given by the following exact solution:

$$u_{\text{exact}}(x,t) = \frac{-\sinh(\frac{x}{2\nu})}{\cosh(\frac{x}{2\nu}) + \exp(-\frac{t}{4\nu})}, \qquad \Omega =]-1, 1[, \quad t \geqslant 0 \tag{17}$$

When the viscosity is very small $\nu \to 0$, a shock appears. Fig. 1 illustrates the behaviour of the numerical solution associated to the implicit Crank–Nicolson scheme (CN scheme) and the explicit invariant FTCS scheme (IFTCS scheme), in comparison to the analytical solution (17). The sizes of the grid are set to $\Delta x = \Delta t = 5 \times 10^{-2}$. The viscosity ν is fixed at 75×10^{-5} (it corresponds to an instability region for the classical FTCS scheme: its solution is completely blown up).

The solution of the CN scheme presents non physical oscillations around high gradient zone. In opposition, the numerical solution of the IFTCS scheme stays close to the analytical solution. Wriggles are avoided but a slight dissipation appears.



(a) FTCS scheme

(b) Invariant FTCS scheme

Fig. 2. Burgers equation. Behaviour of numerical solution of (a): the FTCS scheme, (b): the IFTCS scheme, for different Galilean boost λ. Space step size Δx is 2×10^{-2}. Viscosity ν is 5×10^{-3}. CLF is conserved at $1/2$. Time $t = 2$.

3.2. Galilean invariance

As the set of whole solutions of Burgers equation is invariant under Galilean transformation. The authors test how the numerical solution depends on the referential frame from which it is observed. It is done by the application of a Galilean boost λ to the original referential frame $\Omega =]-2; 2[$. Fig. 2 shows the numerical behaviour of (a): the classical FTCS scheme, and (b): the IFTCS scheme. Space size step is set to $\Delta x = 2 \times 10^{-2}$. Time step size is computed in order to keep the CFL number constant to $1/2$. Viscosity is fixed at $\nu = 5 \times 10^{-3}$. We observe that the solution of the FTCS becomes rapidly degraded as λ grows. The solution blows up when $\lambda \geqslant 1$. It is no more the case when the scheme inherits the property of invariance. The solution remains unaffected irrespective of the value of λ.

4. Conclusion

The authors propose a new approach for construction of invariant numerical schemes using moving frames. This approach is quite different from those proposed by Kim [3], in the sense that the proposed approach is based on numerical rather than geometrical considerations. The advantage of the present method is that it assures good numerical properties in addition to the preservation of the symmetry group of the continuous equation. The application of this method to the explicit FTCS scheme for the Burgers equation yields a stable solution with good accuracy. Invariance has also allowed one to respect the principle of Galilean independence which is broken by the classical scheme.

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