Particle methods revisited: a class of high-order finite-difference schemes

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Abstract

We propose a new analysis of particle method with remeshing. We derive a class of high-order finite difference methods. Our analysis is completed by numerical comparisons with Lax-Wendroff schemes for the Burger equation. *To cite this article: G.-H. Cottet, L. Weynans, C. R. Acad. Sci. Paris, Ser. I 340 (2006).*

Résumé

Les méthodes particulaires revisitées : une classe de schémas de différences finies d'ordre élevé. On propose dans cette note une nouvelle analyse des méthodes particulaires utilisant des remaillages. Cette analyse fait apparaître une classe de schémas de différences finis d'ordre élevé. Des illustrations numériques viennent compléter cette analyse et permettent de comparer les schémas particulaires avec le schéma de Lax-Wendroff. *Pour citer cet article : G.-H. Cottet, L. Weynans, C. R. Acad. Sci. Paris, Ser. I 340 (2006).*

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Méthodes particulaires avec remaillage Les méthodes particulaires (2),(3) sont des méthodes lagrangiennes bien adaptées aux problèmes d'advection de la forme (1). Lorsque le flot subit de fortes distortions, il est souvent conseillé de remailler les particules sur une grille régulière. On considère en général que les remaillages successifs introduisent une erreur de troncature supplémentaire dans l'analyse numérique de ces méthodes. Dans cette note, nous étudions directement les méthodes particulaires avec remaillage à chaque pas de temps. Ceci nous conduit à la construction d'une classe de schémas de différences finies d'ordre élevé que nous analysons dans le cas scalaire.

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Le cas linéaire - Nous considérons d'abord le cas d'une équation d'advection linéaire. Nous nous intéressons aux formules de remaillage construites à l'aide de noyaux d'interpolation (5) conservant les 3 ou 4 premiers moments de la distribution de particules. Nous obtenons selon le cas une schéma de Lax-Wendroff, ou un schéma décentré d'ordre 3.

Le cas non-linéaire - Pour étendre ces résultats au cas non-linéaire, nous sommes conduits à introduire à une méthode originale d'advection des particules, basée sur une évaluation de vitesses utilisant la formule (10), ou sa forme discrète (13). Nous pouvons alors donner une équation équivalente (12) pour le schéma de différences finies associé (11), qui montre en particulier que, pour la formule de remaillage utilisant le noyau Λ_2, la méthode particulaire est d'ordre 2. On montre aussi qu'avec l'adjonction d'un terme de viscosité artificielle approprié l'énergie est une fonction décroissante du temps.

Illustrations numériques - Nous comparons les résultats obtenus par une méthode particulaire et par le schéma de Lax-Wendroff sur l'équation de Burgers (figure 1). Les deux modèles, complétés par les mêmes termes de viscosité artificielle, donnent des résultats semblables. Cependant, la méthode particulaire, au contraire du schéma de Lax-Wendroff, semble converger vers la solution entropique même en l'absence de viscosité artificielle, ce que notre analyse ne permet pas de prévoir. Par ailleurs, de meilleurs résultats pour la méthode particulaire sont obtenus lorsque le pas de temps est adapté au taux de déformation, ce qui illustre une autre différence essentielle avec les schémas de différences finies.

Conclusion - Une nouvelle analyse de méthodes particulaires avec remaillage met en évidence les liens existant entre ces méthodes et des méthodes de différences finies d'ordre élevé. Les méthodes particulaires offrent cependant l'avantage de traiter naturellement des systèmes et le décentrage. L'absence de condition CFL reste aussi une différence notable entre méthodes particulaires et méthodes de différences finies. Cette analyse doit être complétée, notamment pour évaluer les termes de viscosité artificielle optimaux pour ces méthodes.

1. Introduction

Particle methods are Lagrangian techniques that have been designed for advection-dominated physical problems. Among the features that are generally acknowledged for these methodes are the lack of numerical dissipation and the robustness due to the absence of Courant type stability condition. A well recognized drawback is the potential accuracy deterioration resulting form high distortion in the flow. A common remedy to this problem is the periodic remeshing of particles in a way that conserves as much as possible the physical invariants of the flow. Truncation errors related to remeshing can be measured on the basis of the conservation of these invariants [2]. In practical implementation of the method, time-scales wich control the particle advection schemes and on which particle remeshing is done are of the same order, which often leads to remeshing particles at every time-step. In that case, it may be advisable to revisit the truncation error analysis of the method. This is in particular true if one is interested in subgrid behavior of particle methods for turbulent flows or entropy balance in particle methods. The goal of this work is to undergo this analysis in the case of particle methods with remeshing at every time-step. We rewrite particle methods as finite-difference methods. We investigate two remeshing kernels which are commonly used in the literature. In the linear case we show that remeshing with these kernels leads to Lax-Wendroff like schemes [1] . In the non-linear case, this interpretation leads us to propose new RK2 particle advancing schemes. With this time-stepping, we write an equivalent equation to leading order

[1] as we were completing this paper, the reference [3] was brought to our attention. In this reference the authors use the Lax-Wendroff analysis of particle methods to propose modified remeshing kernels.

of the method, which resembles that of Lax-Wendroff schemes. For Burger's equation we are able to derive an energy balance which allows to propose artificial viscosity schemes that enforce energy control. We finally show some numerical comparisons with the Lax-Wendroff scheme to complete our numerical analysis. These preliminary results essentially focus on the 1D case ; extensions to gas dynamics are given in [1] and in ongoing work.

2. Remeshed particle methods

Let us consider the model non-linear scalar equation, describing the evolution of the quantity u carried by the flow at the material velocity $g(u)$:

$$u_t + (g(u)u)_x = 0 \qquad (1) \tag{1}$$

Particle methods consist of sampling u on particles advected with velocity $g(u)$ and constant strength :

$$u(x) \simeq \sum_p \alpha_p \delta(x - x_p) \ , \ \dot{x}_p = g(u_p) \tag{2}$$

The strength of particles combines local volumes v_p and local u values u_p : $\alpha_p = v_p u_p$. Note that, while particle strengths are constant, volumes and local values evolve according to

$$\dot{v}_p = (\partial g(u)/\partial x)(x_p) v_p \ , \ \dot{u}_p = -(\partial g(u)/\partial x)(x_p) u_p \tag{3}$$

In purely lagrangian particle methods, velocities and their derivatives are computed by smoothing particle strength over a space scale containing a *few* particles. The smoothing range must adapt to the flow conditions to smooth out irregular motions [5]. In remeshed particle methods, every *few* time-steps particles are remeshed on a predefined regular grid. Here we consider the case of a uniform grid. Remeshing is done by interpolating particle strength with a kernel Λ with compact support. If $\sum_p \alpha_p \delta(x - x_p)$ and $\sum_q \tilde{\alpha}_q \delta(x - x_q)$ are respectively the original and remeshed particle distribution, with $\tilde{x}_q = qh$ on a regular grid of grid-size h, remeshing formulas read

$$\tilde{\alpha}_q = \sum_p \alpha_p \Lambda(\frac{x_p - \tilde{x}_q}{h}) \tag{4}$$

Conservation of successive moments $\sum \tilde{\alpha}_q = \sum \alpha_p$, $\sum \tilde{x}_q \tilde{\alpha}_q = \sum x_p \alpha_p$, $\sum \tilde{x}_q^2 \tilde{\alpha}_q = \sum x_p^2 \alpha_p \cdots$ can be enforced by using kernels extending to an increasing number of points. The following formulas respectively guarantee conservation of the 3 and 4 first moments and are widely used in CFD :

$$\Lambda_2(x) = \begin{cases} 1 - x^2 & \text{if } |x| \leq 0.5 \\ (1 - |x|)(2 - |x|)/2 & \text{if } 0.5 < |x| \leq 1.5 \\ 0 & \text{if } |x| \geq 1.5 \end{cases} , \ \Lambda_3(x) = \begin{cases} (1 - |x|^2)(2 - |x|)/2 & \text{if } |x| \leq 1 \\ (1 - |x|)(2 - |x|)(3 - |x|)/6 & \text{if } 1 < |x| \leq 2 \\ 0 & \text{if } |x| \geq 2. \end{cases} \tag{5}$$

3. The linear case : $g(u) = a$

We denote respectively by Δt and h the time-step and grid-size. Let us first consider the above 3-points remeshing formula Λ_2, and assume that $\lambda = a\Delta t/h \leq 1/2$. In this case, a particle initially at grid point number p with $x_p = ph$ will after one time-step be remeshed onto 3 particles located at grid points p, $p - 1$ and $p + 1$. If we denote by $\alpha_p^n = h\, u_p^n$ the particle strength at grid-point p and time $t_n = n\Delta t$, we can write

$$u_p^{n+1} = c_0 u_p^n + c_{+1} u_{p+1}^n + c_{-1} u_{p-1}^n \tag{6}$$

The weights c_i determined from the conservation of the 3 first moments must satisfy the following relations :

$$c_{-1} + c_0 + c_{+1} = 1 \ , \ c_{-1} - c_{+1} = \lambda \ , \ c_{-1} + c_{+1} = \lambda^2 \tag{7}$$

from which we readily get $c_0 = 1-\lambda^2, c_{\pm 1} = \mp\lambda(1\mp\lambda)/2$. This is the Lax-Wendroff scheme. If $1 \geq \lambda > 1/2$ one obtains an upwind version of the Lax-Wendroff scheme. Finally if $\lambda > 1$ and if we set $m = [\lambda]$ and $\tilde{t} = mh/a$, the particle method can be interpreted as solving exactly the advection equation from t_n to $t_n + \tilde{t}$ then using one of the above finite-difference schemes from $\tilde{t}$ to t_{n+1}. This reflects the well-known fact that particle methods are not constrained by CFL conditions.

If one now considers the case when we use the function Λ_3 to remesh particles, under the CFL condition $\lambda \leq 1$ we obtain a 4-points upwind finite-difference scheme :

$$u_p^{n+1} = c_0 u_p^n + c_{+1} u_{p+1}^n + c_{-1} u_{p-1}^n + c_{-2} u_{p-2}^n. \tag{8}$$

Conservation of the 4 first moments gives the relations

$$c_{-2} + c_{-1} + c_0 + c_{+1} = 1 \ , \ 2\,c_{-2} + c_{-1} - c_{+1} = \lambda \ , \ 4\,c_{-2} + c_{-1} + c_{+1} = \lambda^2 \ , \ 8\,c_{-2} + c_{-1} + c_{+1} = \lambda^3 \tag{9}$$

The Fourier analysis of this scheme shows that it is third order accurate : if we denote by $\hat{u}_k^n$ the $k-$th fourier mode of the scheme at time t_n we have

$$\hat{u}_k^{n+1} = \hat{u}_k^n [c_0 + c_{-2} \exp(-2ikh) + c_{-1} \exp(-ikh) + c_{+1} \exp(ikh)]$$

and a Taylor expansion in $K = kh$ gives, to third order,

$$\begin{aligned} \hat{u}_k^{n+1} = \hat{u}_k^n \big[& c_{-2} + c_{-1} + c_0 + c_{+1} + (-2c_{-2} - c_{-1} + c_{+1})iK - (4c_{-2} + c_{-1} + c_{+1})K^2/2 \\ & + (8c_{-2} + c_{-1} - c_{+1})iK^3/6 + O(K^4) \big] = \hat{u}_k^n \left[1 - \lambda iK - \lambda^2 K^2/2 + \lambda^3 K^3/6 + O(K^4) \right]. \end{aligned}$$

This is, to third order, the Taylor expansion of the exact solution of the advection equation. This scheme is therefore third order accurate. More generally it is not difficult to see that a particle method with a remeshing formula conserving the p first moments is equivalent to a finite-difference scheme of order p.

4. The non-linear case

Here, for a sake of simplicity, we restrict the discussion to the Λ_2 remeshing formula and we assume that the CFL condition $\Delta t |\max_p g(u_p)| \leq 1/2$ is satisfied. To obtain a second order method in the non-linear case it is clearly necessary to use a second-order time-stepping method to advance particles. In classical implementations of particle methods, particles are moved with *e.g.* Runge-Kutta methods. In a mid-point second order RK time-stepping, particles would be moved for half a time-step, and velocities would be computed at these locations by interpolation and combined with velocities at the beginning of the time-step. Here we propose a different method which is both numerically more efficient and analytically more tractable. To evaluate particle velocity at time $t_n + \Delta t/2$, we use (3) and write

$$u_p^{n+1/2} = u_p^n \left(1 - \Delta t\, g(u)_x(x_p)/2\right). \tag{10}$$

The finite-difference formulas corresponding to this method can be derived along the same lines as in the linear case :

$$u_p^{n+1} = u_p^n - \frac{\Delta t}{2h}(\tilde{g}_{p+1}^n u_{p+1}^n - \tilde{g}_{p-1}^n u_{p-1}^n) + \frac{\Delta t^2}{2h^2}\left((\tilde{g}_{p+1}^n)^2 u_{p+1}^n - 2(\tilde{g}_p^n)^2 u_p^n + (\tilde{g}_{p-1}^n)^2 u_{p-1}^n\right) \tag{11}$$

where we have set $\tilde{g}_p^n = g(u_p^{n+1/2})$.

Proposition 1 *The scheme (10),(11) is second order accurate for smooth solutions. If we set $\mu = \Delta t/h$, its equivalent equation to second order is*

$$u_t + (g(u)u)_x + h^2 \left[\frac{1}{6} (g(u)u)_{xxx} + \frac{\mu^2}{6} u_{ttt} + + \frac{\mu^2}{8} (g(u)_x^2 u^3 g''(u))_x + \frac{\mu^2}{2} \left(g(u)g'(u)u^2 g(u)_x \right)_{xx} \right] = 0 \quad (12)$$

The proof classically relies on Taylor expansions the details of which will be given elsewhere. In practice the calculation of $u_p^{n+1/2}$ is done by finite-difference approximations of the right hand side of (10). We obtain a fully discrete scheme if we replace formula (10) by

$$u_p^{n+1/2} = u_p^n \left[1 - \frac{\mu}{4} \left(g(u_{p+1}) - g(u_{p-1}) \right) \right]. \quad (13)$$

Proposition 2 *The scheme (13),(11) is second order accurate for smooth solutions. Its equivalent equation to second order is (12). Moreover, for the Burger's equation ($g(u) = u/2$) this scheme is energy decreasing when supplemented with an artificial viscosity term of the form $C\mu\Delta_- \left(|\Delta_+ u_j| \Delta_+ u_j \right)$ for $C \geq 0.48$.*

In the above result, we have used the usual notations : $\Delta_\pm f_j = \pm(f_{j\pm1} - f_j)$. The first part of our assertion only results from the fact that the truncation error from the centered approximation of the derivatives of g in (13) only adds third order error terms that do not modify the equivalent equation. Our second assertion comes from lengthy calculations in the spirit of [4]. As a matter of fact the equivalent equations (12) and that of Lax-Wendroff are very similar. However, the numerical results that we show below suggest that their behavior are rather different and that the form of the artificial viscosity proposed in Proposition 2 is not optimal. Note that similar results can be obtained when the remeshing formula Λ_3 is used. The resulting upwind 4-points finite-difference scheme is second order in time and third order in space.

To finish this section, let us comment on the computational complexity of the scheme (13),(11) for multidimensional problems. If u is a scalar or vector quantity and $\mathbf{G}(u)$ is the advection velocity field, to compute $u_p^{n+1/2}$ one must evaluate the divergence of $\mathbf{G}(u)$. This can be easily done by a centered formula using $2d$ points. Although strictly speaking based on a 5 points stencil, the scheme complexity is thus of order $2d + 3^d$, to be compared respectively to 3^d and 5^d for 3-points and 5-points schemes.

5. Numerical illustrations

In this section we complement our numerical analysis with experimental comparisons with the Lax-Wendroff scheme. We considered the Burger's equation with initial condition $u_0(x) = 0$ if $x < 0.5$ and $u_0(x) = 1$ if $x \geq 0.5$. This initial profile produces a shock and an expansion wave that eventually merge together. The top row of figure 1 shows results for the Lax-Wendroff scheme and the particle method with Λ_2 remeshing at two subsequent times. Both calculations used $h = 0.01$, $\mu = 0.8$ and an artificial viscosity coefficient 0.3 produced similar results. The bottom row illustrates the main differences between the two schemes. The left picture shows results without artificial viscosity. These calculations suggest that, unlike the Lax-Wendroff schemes, the particle method, at least in this case, does converge towards the entropy solution, something that the present analysis is not able to predict. The right picture illustrates the fact that particle method are not constrained by CFL conditions. In this calculation, the time step was locally (in space and time) adapted to the local strain in the flow to prevent particles to cross. The corresponding μ varied from 0.07 to 2.5. The artificial coefficient was 0.5. This calculation actually seems to give the best results for the particle method. In all these figures, the solid lines (resp. dotted lines) correspond to the exat (resp. computed) solutions.

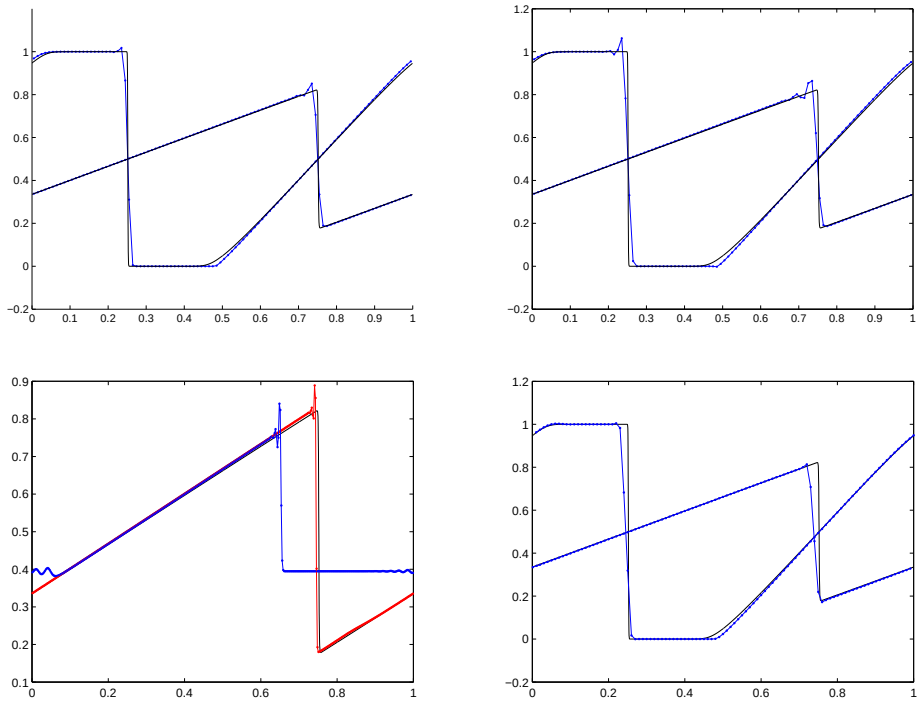

FIG. 1. Comparison of Lax-Wendroff (LW) and particle schemes. Top row : LW (left) and particle (right) schemes with $h = 0.01$, artificial viscosity coefficient 0.2 and $\mu = 0.84$. Bottom left : LW (blue curve) and particle (red curve) schemes without artificial viscosity at $t = 1.5$ and $h = 0.0025$. Bottom right, particle method with adaptive time-step and $h = 0.01$.

6. Conclusion

We have presented a new analysis of particle method with remeshing. We have shown analogies of these method with a class high order finite-difference methods, with however definite advantages for particle methods : natural handling of up-winding through particle advection, simple extensions to system and added flexibility in the choice of time-steps. Further works are needed to continue this analysis and in particular to evaluate the optimal artificial viscosity terms to implement in the particle schemes.

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