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TVD remeshing formulas for particle methods

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Abstract

We derive TVD remeshing formulas for particle methods. The derivation is inspired from a finite-difference analysis but the method retains the essential features of particle methods. Numerical illustrations give evidence of the improved stability and computational cost resulting from these new algorithms. ***To cite this article: G.-H. Cottet, A. Magni, C. R. Acad. Sci. Paris, Ser. I 347 (2009).***

Résumé

Schémas de remaillage TDV en méthodes particulaires. On décrit dans cette Note des techniques de remaillage TVD pour les méthodes particulaires, en s'insipirant de la méthodologie des schémas de différences finies. Des exemples numériques montrent les gains obtenus par ces nouveaux algorithmes tant en stabilité qu'en coût de calcul. ***Pour citer cet article : G.-H. Cottet, A. Magni, C. R. Acad. Sci. Paris, Ser. I 347 (2009).***

Version française abrégée

Méthodes particulaires avec remaillage

Des techniques de remaillage sont souvent utilisées en conjonction avec les méthodes particulaires pour en garantir la précision. Si le remaillage est effectué à chaque pas de temps, on obtient des méthodes de différences finies. L'analyse conduite dans [2] montre que les méthodes particulaires peuvent alors être vues comme des généralisation sans condition CFL de schémas de différences finies multi-dimensionnels. Dans cette Note nous poursuivons cette approche en empruntant aux méthodologies différences finies pour construire des méthodes particulaires TVD.

D'une manière générale les formules de remaillage sont construites pour conserver autant de moments que voulus dans la distribution de particules. La formule générale conservant n moments, et utilisant n points de remaillage en 1D, conduit au schéma (4) (voir aussi la Fig. 1 pour $n = 3$). Dans le cas non-linéaire, il est démontré dans [2] que, pour obtenir l'ordre 2 en temps, il suffit d'évaluer la vitesse des particules grâce à la formule (5). La suite de la Note

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concerne le schéma de remaillage dit Λ_2, correspondant à $n = 3$. L'extension à des formules TVD ou préservant la monotonie d'ordre plus élevé pourra être trouvée dans la référence [4].

Le cas linéaire

Dans le cas linéaire, sous CFL inférieure à un, la formule (6) est équivalente au schéma de Lax–Wendroff. L'utilisation des limiteurs classiques dans ce contexte (voir par exemple [3]) conduit à la formule de remaillage modifiée (9).

Le cas non-linéaire

Dans le cas non-linéaire, le traitement particulaire du flux écrit sous la forme $g(u)u$ nécessite une analyse spécifique pour définir des limiteurs appropriés. En supposant $g \geqslant 0$ et sous CFL 1 une méthode particulaire avec remaillage Λ_2 peut se réécrire sous la forme incrémentale (12). Les calculs sont menés dans le cas de l'équation de Burgers, et permettent de définir de limiteurs à partir des formules (12), (13). Le schéma de remaillage résultant est TVD sous CFL $2/3$.

Illustrations numériques et relaxation de la condition CFL

On commence par un exemple dans le cas non-linéaire, pour l'équation de Burgers. La condition initiale est un créneau périodique qui engendre un choc et une détente se propageant vers la droite. La comparaison de la formule TVD avec le schéma Λ_2 brut (Fig. 1) montre une nette amélioration à la fois dans résolution du choc et de la détente.

On considère ensuite le cas du transport d'un scalaire passif dans un champ de vitesse incompressible. Cet exemple permet d'illustrer le passage au cas multi-dimensionnel, et comment relaxer la condition CFL. L'option choisie est une technique de splitting où les particules sont successivement poussées et remaillées dans chaque direction. Ce schéma n'est plus équivalent à un schéma de différences finies simple mais les limiteurs conservent son caractère TVD. Pour s'affranchir de la condition CFL, une stratégie consiste à définir localement des vitesses uniformes dont ne diffère que de peu la vitesse réelle. La Fig. 2 est une comparaison entre un remaillage TVD Λ_2 à 9 points et la formule à 16 points Λ_3 souvent utilisée en pratique, dans la cas de la rotation dans une boite $[-1, +1]$ d'un disque de rayon 0,1. Cette expérience, menée sous CFL 4, met en évidence à la fois la meilleure qualité des résultats de la méthode TVD et le fait qu'elle génère beaucoup moins de particules, ce qui la rend plus économique.

1. Introduction

Remeshing techniques are often used in conjunction with particle methods for the numerical simulation of advection-dominated problems. These formulas are devised to maintain regularity in the particle distribution. They are necessary to ensure accuracy and have been an essential ingredient for performing reliable DNS of both compressible and incompressible flows. Remeshing techniques are based on interpolation formulas that are designed to conserve a certain number of moments of the particle distribution.

In [2] an analysis of remeshed particle methods was proposed in the framework of finite-difference methods. We in particular proved that remeshed particle methods can be viewed as CFL-free, multidimensional generalization of high order finite-difference methods. Remeshed particle simulations in particular share with high order finite-difference schemes the possible problems related to oscillations. In the present Note, we continue to exploit the analogy between remeshed particle and finite-difference methods to deduce from classical limiters non-oscillatory remeshing formulas for particle methods.

The outline of this Note is as follows. In Section 2 we recall the results of [2]. In Section 3 we derive TVD remeshing formulas for linear and non-linear advection equations. Section 4 is devoted to preliminary numerical illustrations and to a discussion of the CFL number and of the sign independence of the method. Further developments of this approach and applications to gas dynamics, passive advection and incompressible flows will be given elsewhere [4].

2. Previous work

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

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

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

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

The strengths of the particles combine 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

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

In remeshed particle methods, every *few* time-steps particles are remeshed on a predefined regular grid. New particles at locations x_p with strengths α_p are obtained from old particles $\tilde{x}_p$, $\tilde{\alpha}_p$ resulting form advection by the following general formula $\alpha_p = \sum_q \tilde{\alpha}_q \Lambda(x_p - \tilde{x}_q)$. The accuracy of remeshing is governed by the conservation of successive moments $\int x^m u(x)\, dx$ of the particle distribution which can be enforced by increasing the size of the support of the kernel Λ [1].

In [2] an analysis of remeshed particle methods is done on the basis of their analogy with finite-difference schemes. Let us consider the case when particles are remeshed at every time-step (we will call this particle method "push-and-remesh") with a remeshing formula preserving the n first moments of the particle distribution. In the case of a linear advection equation, $g(u) = a$, with constant advection velocity $a > 0$, when $a\Delta t \leqslant h$, if a particle initialized at ih is located at x after an advection step, one has $\lambda = \frac{x-ih}{h} = a\Delta t/h$ and we obtain the following scheme:

$$u_i^{n+1} = \sum_{-[\frac{n-1}{2}]\leqslant j\leqslant[\frac{n}{2}]} w_j u_{i-j}^n, \quad w_j = c_k \prod_{-[\frac{n-1}{2}]\leqslant k\neq j\leqslant[\frac{n}{2}]} (\lambda - k), \tag{4}$$

where $c_k = (-1)^{[\frac{n-1}{2}]+k}([\frac{n-1}{2}] + k)!([\frac{n}{2}] + k)!$. Not surprisingly, we obtain general finite-difference formulas for the linear advection equation [5]. For $n = 3$ we obtain $w_0 = 1 - \lambda^2$, $w_{\pm 1} = \mp\lambda(1 \mp \lambda)/2$ – the Lax–Wendroff scheme. Following [1], we will call this scheme the left-Λ_2 remeshing scheme.

In the more general non-linear case (1), the link with finite-difference methods is not as direct and we do not recover *classical* finite-difference formulas. It is proved in [2] that if particle velocities are evaluated at time t_n by the formula

$$u_j^{n+1/2} = \tilde{g}\big(u_j^n\big) = g\left(u_j^n\left[1 - \frac{\Delta t}{4h}\big(g\big(u_{j+1}^n\big) - g\big(u_{j-1}^n\big)\big)\right]\right), \tag{5}$$

the push-and-remesh scheme (4) with $n = 3$ and $\lambda_j = \tilde{g}(u_j^n)\Delta t/h \leqslant 1$ is equivalent to a stable second-order (both in space and time) finite-difference scheme. For a sake of clarity we denote by α_i, β_i, γ_i the weights in formula (4), associated to grid points from left to right (see Fig. 1) for the left-Λ_2 remeshing, which thus reads:

$$u_i^{n+1} = u_{i-1}^n \gamma_{i-1} + u_i^n \beta_i + u_{i+1}^n \alpha_{i+1}. \tag{6}$$

3. TVD remeshing formulas

In this section we show how finite-difference inspired limiters allow to construct TVD remeshing formulas. We here restrict ourselves to the case $n = 3$ and refer to [4] for higher order TVD and Monotony Preserving formulas.

3.1. The 1D, linear, constant-coefficient, case

We first consider the case $g(u) = a$, $a > 0$, and set $\lambda = a\Delta t/h$ and $\Delta u_{i+1/2} = u_{i+1} - u_i$. We start from classical flux-limited versions of the Lax–Wendroff scheme [3]:

$$u_i^{n+1} = u_i^n - \lambda(u_i - u_{i-1}) - \lambda(1 - \lambda)(\phi_{i+1/2}\Delta u_{i+1/2} - \phi_{i-1/2}\Delta u_{i-1/2})/2, \tag{7}$$

where

$$\phi_{i+1/2} = \phi(r_{i+1/2}), \quad r_{i+1/2} = \frac{u_i - u_{i-1}}{u_{i+1} - u_i}. \tag{8}$$

This gives the limited left-Λ_2 remeshing formula (6) with

$$\alpha_{i+1} = -\frac{\lambda}{2}(1-\lambda)\phi_{i+1/2}, \qquad \beta_i = 1 - \lambda + \frac{\lambda}{2}(1-\lambda)(\phi_{i-1/2} + \phi_{i+1/2}), \qquad \gamma_{i-1} = \lambda - \frac{\lambda}{2}(1-\lambda)\phi_{i-1/2}. \tag{9}$$

By Harten's theorem [3], this remeshing scheme is TVD under the condition $|\phi(r)/r - \phi(s)| \leqslant \Phi$ with:

$$1 - (1-\lambda)\Phi/2 \geqslant 2, \qquad 1 + (1-\lambda)\Phi/2 \leqslant 1/\lambda.$$

If $a < 0$, the remeshing formula is equivalent to a Beam–Warming upwind. One can then show, and this is important from a practical point of view, that Eq. (9) can still be used to determine the remeshing weights. This property will be illustrated below in the example of a rotating patch.

3.2. *The non-linear case*

We consider Eq. (1) and the push-and-remesh method with left-Λ_2 remeshing, with particle velocities evaluated through (5). We assume here that $\tilde{g} > 0$ and set $\nu = \Delta t/h$, $\tilde{f}_j = \tilde{g}_j u_j$, $h_j = \tilde{f}_j(1 - \nu\tilde{g}_j)$.

The push-and-remesh method can then be rephrased as the following centered finite-difference scheme

$$u_i^{n+1} = u_i^n - \nu\Delta\tilde{f}_i - \nu(\Delta h_{i+1/2} - \Delta h_{i-1/2})/2. \tag{10}$$

We look for a TVD modification of the above scheme under the form

$$u_i^{n+1} = u_i^n - \nu\Delta\tilde{f}_i - \nu(\phi_{i+1/2}\Delta h_{i+1/2} - \phi_{i-1/2}\Delta h_{i-1/2})/2, \tag{11}$$

from which the remeshing weights can be recovered using (9). Because of the way particle methods handle fluxes, we need a specific derivation of the limiter ϕ that we outline here. We set $r_{i+1/2} = \Delta h_{i-1/2}/\Delta h_{i+1/2}$ so that (11) can be rewritten in incremental form

$$u_i^{n+1} = u_i^n - \Delta u_{i-1/2} D_{i-1/2}, \quad D_{j-1/2} = \nu\frac{\Delta h_{i-1/2}}{\Delta u_{i-1/2}}\left[\frac{\Delta f_{i-1/2}}{\Delta h_{i-1/2}} + \frac{1}{2}\left(\frac{\phi_{i+1/2}}{r_{i+1/2}} - \phi_{i-1/2}\right)\right]. \tag{12}$$

To obtain a TVD scheme we need to construct ϕ such that $0 \leqslant D_{i+1/2} \leqslant 1$ under some CFL conditions. We derive these conditions below in the particular case of the Burgers equation $g(u) = u/2$, with $u > 0$. We set $\lambda = \nu \max|u|$ and we further assume the usual CFL condition $\lambda \leqslant 1$.

We have $f'(u) = u$, $h'(u) = u(1 - 3u/4)$ so that $\Delta h_{i-1/2}/\Delta u_{i-1/2} \geqslant 0$, $\Delta f_{i-1/2}/\Delta h_{i-1/2} \geqslant 0$. Moreover

$$\left|\frac{\Delta h_{i-1/2}}{\Delta u_{i-1/2}}\right| \leqslant \lambda(1 - 3\lambda/4) \leqslant 1/3, \qquad \left|\frac{\Delta f_{i-1/2}}{\Delta h_{i-1/2}}\right| \leqslant \frac{1}{1 - 3\lambda/4}$$

so that the scheme (12) is TVD, provided the function ϕ satisfies (see [3])

$$\left|\frac{\phi(r)}{r} - \phi(s)\right| \leqslant \Phi, \qquad \frac{1}{1 - 3\lambda/4} + \frac{\Phi}{2} \leqslant 3, \qquad \frac{1}{1 - 3\lambda/4} - \frac{\Phi}{2} \geqslant 0. \tag{13}$$

It is readily checked that the value $\Phi = 2$ is allowed provided the CFL condition is reduced to $\lambda \leqslant 2/3$. In that case, the usual TVD limiters, such as Van-Leer or Superbee can be used.

4. Numerical illustrations, sign independence and extension to CFL larger than 1

We first consider the Burgers equation. The initial condition is a step function in $[-1, +1]$, $u_0(x) = 0$ if $x \leqslant 0$, $u_0(x) = 1$ otherwise, with periodic boundary conditions. It develops a shock and a rarefaction wave propagating to the right.

Fig. 1 shows the solution obtained at $t = 0.8$ for the original and TVD Λ_2 remeshing, for $h = 0.02$ and a CFL number $2/3$. The TVD remeshing formula used a Van-Leer limiter. The TVD remeshing formula removes the oscillations. Note that, unlike the Lax–Wendroff scheme, the remeshed particle method satisfies the entropy condition, an important property which remains to be rigorously proved.

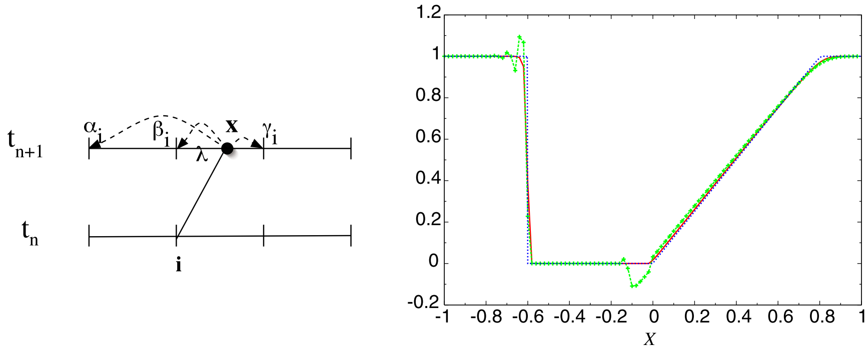

Fig. 1. Left picture: sketch of push-and-remesh Λ_2 scheme. Right picture: simulation of the Burgers equation; original (green crosses) or TVD (red continuous line) remeshing schemes compared to exact solution (blue dotted lines).

We continue with the linear case of the passive transport of a scalar in a 2D incompressible flows. Although it does not enter the general case, this case is useful to illustrate how the TVD formulas are extended to the multidimensional case and how the CFL condition can be relaxed. To deal with advection in a multidimensional field, the approach we choose follows the classical splitting used in finite-difference methods. In a push and remesh methods, it means that particles are advected in one direction, then remeshed, then advected in a second direction and so on. This is clearly a first order in time method and higher order strategies can be devised as for classical differential equations. Note that this method, for not constant velocity values, is no longer equivalent to a finite-difference method, because particle in the second and following advection stages "see" velocity values at the location where they have been remeshed.

In this experiment we consider the evolution of a circular patch in a rotating rigid velocity field. We used a splitting method together with the left-Λ_2 TVD remeshing after advection of particle in each direction. In this example we used the Superbee limiter. As announced earlier, despite the sign changes we were able to use the same remeshing weights at all particle locations. The derivation of the TVD remeshing formulas is based on the assumption of a CFL number less than 1. However one specific feature of particle methods is that they are CFL free, which often enables to use much larger time-step than for Eulerian methods. It is therefore very much desirable to relax the CFL condition for the TVD remeshing formulas. The CFL condition is clearly not necessary for the constant velocity case, because in this case particles conserve their slopes during advection. One way to relax the CFL condition in the general case is to determine zones of the flow where the velocity is close to a constant value. If $a(x) = \bar{a} + \tilde{a}(x)$, and if Δt is such that $\bar{a}\Delta t = Nh$ and $\max|\tilde{a}|\Delta t \leqslant h$, the idea is to advect particles with $\bar{a}$, without remeshing, and to follow this advection with a push-and-remesh TVD method. This algorithm will be given in more details in [4]. In the present example, a CFL number equal to 4 could be used by partitioning the computational domain in 16 boxes.

Fig. 2 shows, for the left-Λ_2 TVD scheme, using 3 grid points, and the original Λ_3 scheme using 4 grid points, a cross-section and contours of the patch after one turn. The patch had a radius of 0.1. The particle spacing was 0.01. For a better comparison we have translated the patch obtained by the TVD remeshing formulas by 0.25 in the vertical direction. This figure illustrates the improved accuracy obtained by TVD formulas. It also shows the time-evolution of the number of particles, initially located inside the patch. In practice, at the end of the remeshing step, particles having a strength less than a given cut-off (say 10^{-6} times the maximum value) are discarded. The number of particles generated by the TVD formula is remarkably lower than for the original Λ_3 remeshing formula. In this example the TVD formula is much less expensive by the combined effects of the following factors: it generates less particles and it uses a smaller stencil (3 points instead of 4). Moreover, one can observe that the splitting strategy is by itself less expensive than the traditional remeshing strategy: in 3D, for a Λ_2 formula, the cost of the splitting method is O(9N) instead of O(64N) for a regular Λ_3 formula.

5. Conclusion

We have introduced a methodology inspired from finite-difference methods to design TVD remeshing formulas for the simulation of advection-dominated problems by particle methods. We have shown that these methods can retain the important features of particle methods with respect to localization and time-step limits. Preliminary validations illustrate the gain offered by the new remeshing formulas not only in stability but also in computational cost.

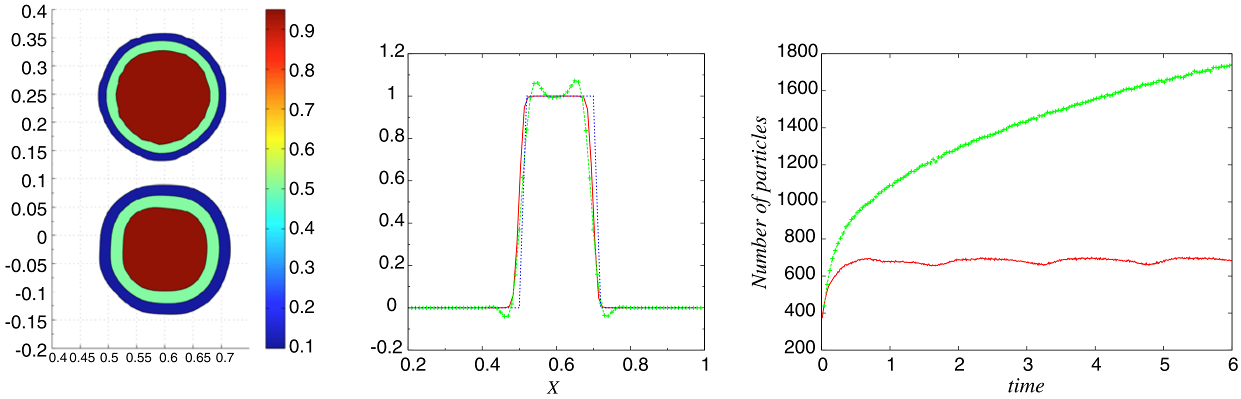

Fig. 2. Passive transport of circular patch in a rigid vorticity field, after one turn. Left picture: contours for values 0.1, 0.5 and 0.95. Middle picture: cross sections. Right picture: time evolution of the number of particles. Green crosses: classical Λ_3 remeshing; red continuous line: TVD Λ_2; blue dotted line: exact solution.

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