New space staggered and time interleaved 2^{nd} order finite volume methods

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Summary. A new modified version of the Nessyahu-Tadmor (NT) 1-dimensional finite volume central scheme is presented , as well as corresponding new versions for 2D-structured and 3D-unstructured grids inspired from the NT scheme. The modification avoids the intermediate predictor time step between t^n and t^{n+1}.The CPU gain is not very important in the 1D case, but becomes significant in the 2 and 3D cases. 3D comparative simulations for the shock tube problem and for a supersonic inviscid flow through a channel with a 4% circular bump are presented.

1 Introduction

We consider central methods for scalar hyperbolic conservation laws or corresponding systems:

$$u_t + f(u)_x = 0, \qquad u(x, t = 0) = u_0(x) \tag{1}$$

as well as their 2 and 3-dimensional analogue, to be described below. The non-oscillatory central difference scheme of Nessyahu and Tadmor may be interpreted as a Godunov-type scheme for one-dimensional hyperbolic conservation laws in which the resolution of the Riemann problems at the cell interfaces is by-passed thanks to the use of the staggered Lax-Friedrichs scheme. Piecewise linear MUSCL-type cell interpolants and slope limiters lead to an oscillation-free second-order resolution.

In earlier papers [5, 7, 6] a two- dimensional finite volume method was presented, generalizing the one-dimensional Lax-Friedrichs (LF) and Nessyahu - Tadmor (NT) [12] difference schemes for hyperbolic conservation laws to unstructured triangular grids, while in [3, 4] a corresponding extension in the case of 2-dimensional Cartesian grids was constructed. In [9], Jiang and Tadmor have presented a slightly different extension for Cartesian grids.

In [2, 4] new extensions of the LxF and NT schemes to central finite volume methods for 3-dimensional hyperbolic systems on **unstructured tetrahedral grids** and on **Cartesian grids**, respectively, were presented.

In this paper, we investigate another way to improve our 2 and 3-dimensional

central finite volume methods inspired from the LF and NT schemes. These methods require the implementation of an intermediate half-time predictor step to compute the fluxes with the midpoint rule. Since the execution of this predictor step becomes more and more time consuming in 2 and 3D, we present a variant of our schemes which avoids the predictor step. The new method is inspired by multistep methods for ODE's, and computes the fluxes with the help of the values of the dependent variables at the last two time steps. Since the NT scheme and our finite volume extensions use two staggered grids at alternate time steps, the solution at time t^{n+1} is constructed using the fluxes at t^n and t^{n-2}, both obtained from the same grid.
Although the new method does not lead to significant computer time reduction in the one dimensional case, it really becomes advantageous in two and even more so in three spatial dimensions, where it can lead to reductions up to 40% in total computer times.

2 The 1D NT-type scheme without predictor step

2.1 The Lax-Friedrichs and Nessyahu-Tadmor difference schemes

We consider the initial value problem (1) and the staggered LF scheme

$$u_{i+1/2}^{n+1} = \frac{1}{2}(u_{i+1}^n + u_i^n) - \lambda(f(u_{i+1}^n) - f(u_i^n)) \qquad (\lambda \equiv \frac{\Delta t}{h} \equiv \frac{\Delta t}{\Delta x}) \tag{2}$$

Starting from initial values

$$u_i^0 = \frac{1}{h}\int_{x_{i-1/2}}^{x_{i+1/2}} u_0(x)dx \tag{3}$$

the first (or further odd) time step of (2), with $n = 0$ (or $n = 2n'$,$n' = 1, 2, ...$) leads to staggered values $\{u_{i+1/2}^1\}$ (or $\{u_i^{2n'+1}\}$) which can be considered as piecewise constant on the cells $C_{i+1/2}$ of the staggered, dual grid:

$$C_{i+1/2} = \{x | x_i = ih < x < x_{i+1}\} \tag{4}$$

To obtain second-order accuracy, Nessyahu and Tadmor [12] introduced van Leer's MUSCL-type [16] piecewise linear reconstruction of the piecewise constant solution obtained at the previous step:

$$u(x, t^n) = L_i(x, t^n) = u_i^n + (x - x_i)\frac{u_i'}{\Delta x} \quad x \in C_i \tag{5}$$

where

$$u_i' = (u_i^n)' \cong h\frac{\partial}{\partial x}u(x, t^n)|_{x=x_i} + O(\Delta x^2) \tag{6}$$

Integrating (1) on $[x_i, x_{i+1}] \times [t^n, t^{n+1}]$ and using Green's formula gives

$$\int_{x_i}^{x_{i+1}} u(x,t^{n+1})dx = \int_{x_i}^{x_{i+1}} u(x,t^n)dx - \{\int_{t^n}^{t^{n+1}} f(u(x_{i+1},t))dt - \int_{t^n}^{t^{n+1}} f(u(x_i,t))dt\} \quad (7)$$

Applying the midpoint rule to the flux integrals then leads to the NT formula:

$$u_{i+1/2}^{n+1} = \frac{1}{2}(u_{i+1}^n + u_i^n) + \frac{1}{8}((u_i^n)' - (u_{i+1}^n)') - \lambda(f(u_{i+1}^{n+1/2}) - f(u_i^{n+1/2})) \quad (8)$$

where $u_i^{n+1/2}$ is an approximate value defined by a **predictor step**[12].

2.2 One-dimensional NT-type scheme without predictor step

Instead of using the (NT)-predictor to obtain second order time accuracy, the flux function will be reconstructed with the help of previous values. We start from (7) and denote by $\mathcal{P}(x,t)$ the first degree Lagrange polynomial interpolating the function $f(u(x,t))$ at the nodes t^{n-2}, t^n (considering x as a parameter). Integrating $\mathcal{P}(x,t)$ instead of $f(u(x,t))$ in (7) leads to our modified form of the NT scheme

$$u_{i+1/2}^{n+1} = \frac{1}{2}(u_{i+1}^n + u_i^n) + \frac{1}{8}((u_i^n)' - (u_{i+1}^n)') - \frac{\Delta t^{n+1}}{h}\{\mathcal{F}(u_{i+1}^n, u_{i+1}^{n-2}) - \mathcal{F}(u_i^n, u_i^{n-2})\} \quad (9)$$

where

$$A_1 = 1 + \frac{\Delta t^{n+1}}{2(\Delta t^{n-1} + \Delta t^n)}, \quad A_2 = 1 - A_1 \quad (10)$$

and $\Delta t^n = t^n - t^{n-1}$, and where

$$\mathcal{F}(u_i^n, u_i^{n-2}) \equiv A_1 f(u_i^n) + A_2 f(u_i^{n-2}) \quad (11)$$

is a modified numerical flux inspired by multistep methods for ODE's.

3 2D and 3D NT-type FV methods without predictor

Starting from the following model equation ($\mathbf{F} : \mathbb{R} \mapsto \mathbb{R}^{(2,3)}$):

$$u_t + \nabla \cdot \mathbf{F}(u) = 0, \;\; u(\mathbf{x}, 0) = u_0(\mathbf{x}) \quad (12)$$

we rewrite (12) in a method of lines fashion:

$$u_t = -\nabla \cdot \mathbf{F}(u) \equiv G(u) = \frac{\partial u}{\partial t} \tag{13}$$

In the original finite volume formulation for tetrahedral grids, (12) is integrated with respect to space on the dual cells L_{ij} and from t^n to t^{n+1} (Fig. 1). Instead of $G(u)$ we integrate its $\mathcal{P}_1$-Lagrange polynomial:

$$\mathcal{P}(\mathbf{x},t) =\left(\frac{(t-t^{n-2})G(u(\mathbf{x},t^n))}{\Delta t^n + \Delta t^{n-1}} + \frac{(t^n - t)G(u(\mathbf{x},t^{n-2}))}{\Delta t^n + \Delta t^{n-1}}\right) \tag{14}$$

First, integrating by parts with respect to time leads to

$$\int_{L_{ij}} u(x,t^{n+1})dV = \int_{L_{ij}} u(x,t^n)dV + \int_{L_{ij}} \int_{t^n}^{t^{n+1}} \mathcal{P}(\mathbf{x},t)dtdV + O(\Delta t)^2 \tag{15}$$

Proceeding as in section 2 for the cell values $u_{L_{ij}}(t^n) = u^n_{L_{ij}}$, then gives

$$\begin{aligned} u_{L_{ij}}(t^{n+1})vol(L_{ij}) = &\int_{L_{ij}\cap C_i} u(x,t^n)dV + \int_{L_{ij}\cap C_j} u(x,t^n)dV \\ &+ \int_{L_{ij}} \{A_1 G(u(\mathbf{x},t^n)) + A_2 G(u(\mathbf{x},t^{n-2}))\}dV \end{aligned} \tag{16}$$

with A_1, A_2 given by (10). Applying the divergence theorem leads to

$$\begin{aligned} u_{L_{ij}}(t^{n+1})vol(L_{ij}) = &\int_{L_{ij}\cap C_i} u(x,t^n)dV + \int_{L_{ij}\cap C_j} u(x,t^n)dV \\ &-\left(\int_{\partial L_{ij}\cap C_i} + \int_{\partial L_{ij}\cap C_j}\right)\{A_1\mathbf{F}(u(\mathbf{x},t^n)) + A_2\mathbf{F}(u(\mathbf{x},t^{n-2}))\}\cdot \hat{n}dA \end{aligned} \tag{17}$$

which represents the **NT-type finite volume method without predictor** in its version valid for **3-dimensional unstructured tetrahedral grids**. Fig. 1 shows the part of the cell C_i (centered at node i) which is contained in the tetrahedron $ijkl$, and the dual cell L_{ij} constructed about the edge ij.

4 Stability

The study of stability for our new scheme (9) is more difficult than for the NT scheme. We have used a heuristic CFL condition obtained by multiplying by $\frac{1}{A_1}(\equiv \frac{4}{5}$ in the case of constant $\Delta t)$ the maximum CFL number used in the case of the corresponding schemes without occurrence of the values at time t^{n-2}. For instance, since the NT scheme is TVD for

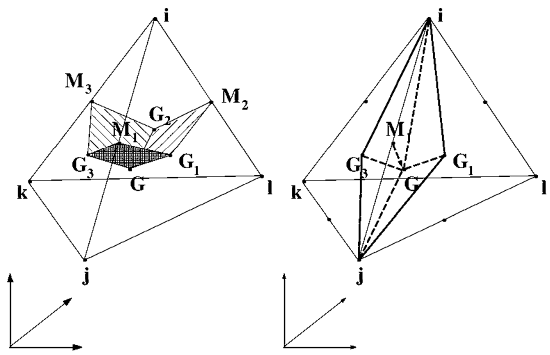

Fig. 1. Barycentric cell C_i and diamond cell L_{ij}

$$\lambda \max_i |f'(u_i)| \leq \beta, \quad \text{with} \quad \beta \leq \frac{1}{2}, \tag{18}$$

we have used a CFL number of the order of $\frac{4}{5} \cdot \frac{1}{2} = \frac{2}{5}$. Considering now the unstructured tetrahedral 3D case, recalling the original scheme presented in [2], for the Euler equations, and applying the condition for a monotone scheme $\frac{\partial H}{\partial u_j^n} \geq 0$, we had been using the following time step for the scheme with predictor

$$\Delta t_i = \frac{Vol(C_i)}{\lambda^i_{max} \displaystyle\int_{\partial C_i} d\sigma}$$

where

$$\lambda^i_{max} = \max(\lambda_i, \max_{j \in \mathcal{N}(i)} \lambda_j) \quad \text{and} \quad \lambda_i = ||\overrightarrow{V}_i|| + c_i$$

and $\overrightarrow{V}_i$, c_i refer to the values in the cell C_i of the velocity vector and sound speed, respectively. We chose the minimum Δt_i for all cell indices i : $(1 \leq i \leq nv)$ $\Delta t = \min\limits_{1 \leq i \leq nv} \{\Delta t_i\}$. We then used the multiplier $\frac{4}{5}$ to obtain our time step for the new scheme.
For a more detailed discussion of stability, consult Shu [13] and a forthcoming paper.

5 Numerical results

In all structured tests the *minmod-2* limiter (consult [12] p. 418) was used, while on unstructured 3D grids for the shock tube problem the new Venkatakrishnan limiter was applied. For the bump problem, van Leer's limiter was used because of its low computational cost. For details on those limiters, one can consult [16, 17, 4, 9]. It is worth mentioning that no artificial compression was applied on the NT scheme in any dimensions. Doing so would greatly improve the quality of the solution, particularly for the contact discontinuities, and could be applied to all of the newly proposed methods.

5.1 Cartesian 2D

Solving again Sod's shock tube problem [14] extended to 2 spatial dimensions and taking a transverse cut in the 2D plane gives the densities shown on figures (2) (to be compared with the results of the 1D scheme). The results are very similar for both schemes and generally good, except for the contact discontinuity which is somewhat smeared.

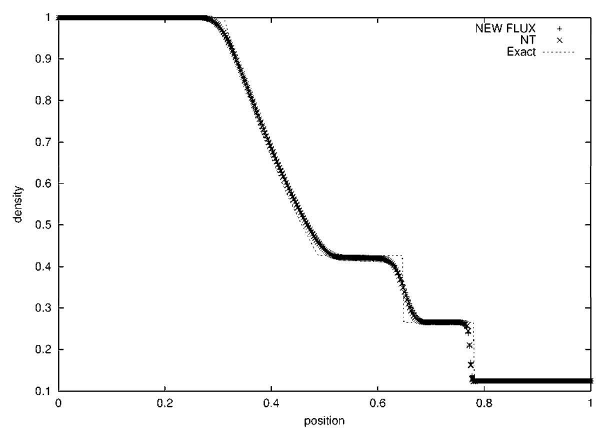

Fig. 2. Sod's shock tube 2D N=400 at $t = 0.16$

5.2 Unstructured 3D

Shock tube For comparison purposes, the shock tube problem is again solved here by applying the unstructured tetrahedral 3D schemes. Resulting densities obtained respectively by the use of the Nessyahu-Tadmor-like scheme (with predictor) and with the new proposed (faster) scheme (without predictor) are given in Fig.3. As in the 2-D case, the results for both schemes are practically indistinguishable. Here in 3D, the cost of performing the half time step is significant since 3 matrix-vector multiplications are needed at each node. The order of convergence of the scheme has been observed to be only 1.22 for nonlinear systems in [2], which has been confirmed by the recent theoretical results of [11] for a truly nonlinear scalar equation.

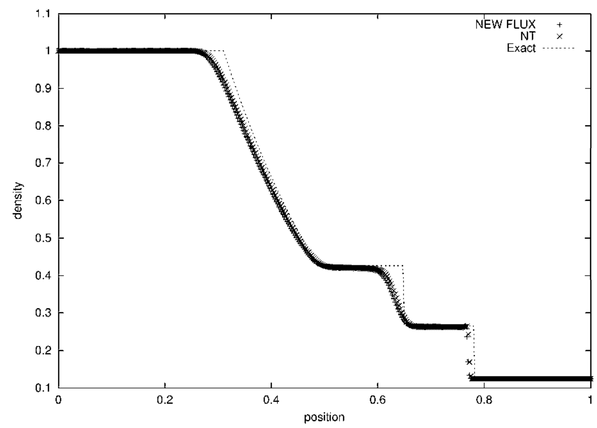

Fig. 3. Sod's shock tube 3D N=400 at $t = 0.16$

Channel with a 4% circular arc bump with $M_\infty = 1.65$ *Original 3D-unstructured Scheme*

An inviscid supersonic flow is considered over a circular 4% arc bump; this test case was first proposed as a benchmark problem by Eidelman et al. [8].The left boundary of the computational domain is considered as the inlet of the flow with a prescribed supersonic condition, namely : $(\rho, u, v, w, p) = (1.4, 1.65, 0, 0, 1)$ and the right boundary is considered as a supersonic outlet. For the sake of comparison 3 different meshes were used with 18079, 64099 and 138561 tetrahedra, respectively. For simplicity, we only show the results obtained with the final grid, which has a characteristic length of 1/30, 23279 nodes and 154535 edges (fig. 4). The results are comparable with those of the structured cases presented in [10] since the numbers of unknowns are about the same. An interesting property of the new scheme is the convergence rate to the stationary solution (Fig.6); the single precision machine epsilon is reached without requiring any special limiter like the one proposed by Venkatakrishnan, hence preventing any over/undershoot as observed in [1, 10].
3D-unstructured Interleaved Scheme

The new scheme does not need an predictor step as required by the original unstructured scheme proposed in [2]. Since the scheme is explicit and both edge based and vertex based data structures are used, the gain is evaluated on a tetrahedron basis (second/(cell $\times$ iteration)). The original scheme requires 2.5×10^{-5} second while the interleaved scheme requires only half of that time i.e. 1.25×10^{-5} second/(cell $\times$ iteration). This acceleration is directly reflected in the calculations since it is possible to use twice as many cells and

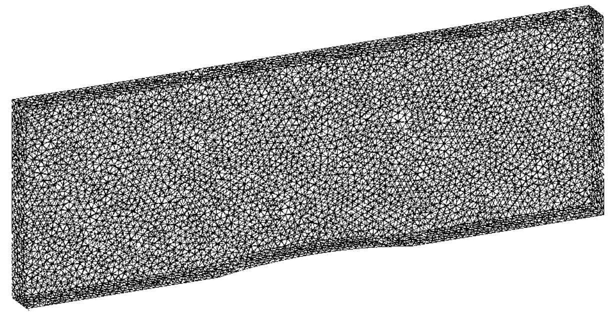

Fig. 4. Final mesh with characteristic length 1/30 (138561 Tetrahedra)

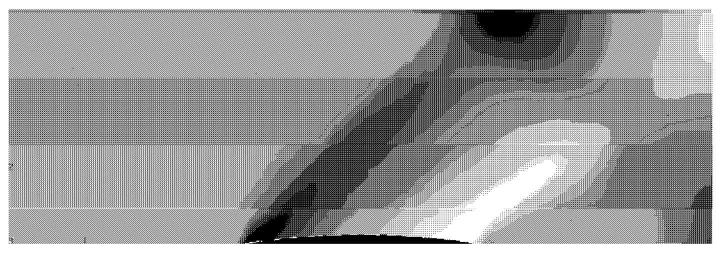

Fig. 5. Isomach lines (138561 Tetrahedra)

obtain a substantially finer solution in about the same time as that needed for the first method to solve the problem on a coarser mesh. The results are practically indistinguishable from those obtained with the scheme with predictor, so that Fig.5 is valid for both schemes. A plot of the isomach lines is given in Fig.6. As regards convergence to the steady state, the machine tolerance is reached in less than 2000 iterations for the original scheme, and 2500 iterations for the new scheme. Despite the fact that the CFL condition used with the interleaved scheme is more restrictive, thus requiring more time steps to reach the stationary state, the computing times are reduced by approximately 37% (Table 1).

Mesh 3 (138561 Elements)	iterations	time(sec)	Normalized
Original Scheme	1692	5868	1.00
Interleaved Scheme	2123	3681	0.63

Table 1. Comparison of the two schemes for a fixed residual

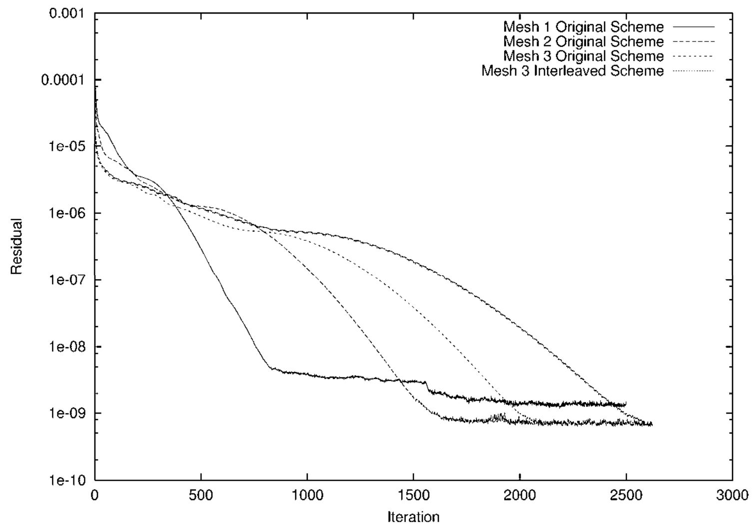

Fig. 6. Convergence history (residuals)

6 Conclusion

We have presented a new structured and unstructured Riemann solver-free centered finite-volume method for solving systems of conservation laws in 1,2 and 3D. The new scheme is significantly faster for 2 and 3D systems. The resolution is comparable in all dimensions with that of the NT scheme and its 2 and 3D extensions. This makes the new scheme computationally more efficient while being comparable, for accuracy, with the NT scheme and its 2 and 3D finite volume extensions for Cartesian or unstructured grids. The authors would like to thank J. F. Remacle at Rensselaer Polytechnic Institute for the freely available mesh generator GMSH.

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