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Fast high order ADER schemes for linear hyperbolic equations

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Abstract

A reformulation of the ADER approach (Arbitrary high order schemes using DERivatives) for linear hyperbolic PDE's is presented. This reformulation leads to a drastic decrease of the computational effort. A formula for the construction of ADER schemes that are arbitrary high order accurate in space and time is given. The accuracy for some selected schemes is shown numerically for the two-dimensional linearized Euler equations as a mathematical model for noise propagation in the time domain in aeroacoustics. © 2003 Elsevier Inc. All rights reserved.

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1. Introduction

Finite volume schemes have become very popular in computational fluid dynamics due to their robustness and flexibility. They consist of two steps: the reconstruction and the flux calculation. The discrete values are approximations of cell averages. By the reconstruction step, local values are interpolated from the average values to calculate the numerical flux between the grid cells. The construction of high order schemes concerning spatial discretization has been introduced with the idea of ENO and WENO interpolation [4,5]. But the time integration usually becomes a limiting factor for accuracy. All these schemes are generally discretized in time with Runge–Kutta (RK) schemes. These time integration schemes become inefficient for orders of accuracy higher than four. It can be proven, that all explicit RK time integration schemes of order higher than four need more integration stages than their order. This is the so-called Butcher barrier [2].

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The idea of the ADER approach of Toro (see, e.g., [7,9,11]) is to circumvent this efficiency barrier for the time discretization by considering finite space-time volumes, where the temporal evolution of the fluxes over the borders of the finite volumes is estimated by a Taylor series in time. The time derivatives are then replaced by space derivatives using the Lax–Wendroff procedure. With this approach it is (at least theoretically) possible to construct schemes of arbitrary high order in space and time with $\Delta t \sim \Delta x$ close to the stability limit. However, the Lax–Wendroff procedure becomes cumbersome already in the case of linear systems of PDE's for very high order ADER schemes. If the ADER approach is applied without any special treatment, it is not competitive with e. g. finite difference schemes for the solution of linear PDE's with respect to the computational effort. In this paper we develop a particular formulation of the ADER approach, which makes use of simplifications that can be taken into account for linear PDE's on structured meshes. A typical field of application would be computational aeroacoustics to simulate noise propagation in the time domain or electromagnetic wave propagation.

The scope of the paper is as follows. In Section 2 we first give the formulas which are essential for the reformulation. We derive then a finite difference-like formulation of the ADER approach which significantly enhances efficiency with respect to computational effort. In Section 3 we show the convergence rates obtained with the reformulated ADER schemes in numerical experiments for the two-dimensional linearized Euler equations up to 16th order of accuracy in space and time.

2. The fast-ADER approach

The ADER approach is a scheme developed to calculate numerical solutions of systems of hyperbolic PDE's up to an, at least theoretically, arbitrary order. Toro and Millington [11,13] first developed the idea in one space dimension. Here, the 1st order scheme reduces to the Godunov scheme and the 2nd order scheme is equivalent to the MGRP approach by Toro [12,13], which is a simplified GRP scheme of Ben-Artzi and Falcovitz [1]. The extension to multi-dimensions is straightforward and can be found in [7–9]. In the following we shortly review the basic steps and then we reformulate the whole procedure to obtain an efficient algorithm. A general system of linear hyperbolic PDE's in two dimensions is given by

$$\vec{U}_t + \underline{\underline{A}}\vec{U}_x + \underline{\underline{B}}\vec{U}_y = 0, \quad \vec{U} = \vec{U}(x, y, t) \quad \text{and} \quad \vec{U}(x, y, 0) = \vec{U}^0(x, y), \tag{1}$$

where \vec{U} denotes the vector of physical variables and the matrices $\underline{\underline{A}}$ and $\underline{\underline{B}}$ are assumed to be constant. The physical fluxes \vec{F} and \vec{G} are determined by

$$\vec{F} = \underline{A}\vec{U}$$
 and $\vec{G} = \underline{B}\vec{U}$. (2)

Consider now a space-time element $I_{ij} \times [t^n, t^{n+1}]$ as a control volume. The integration of the conservation Eq. (1) over this control volume gives the evolution equations for the cell averages as

$$\overline{\vec{U}}_{ij}^{n+1} = \overline{\vec{U}}_{ij}^{n} - \frac{\Delta t}{|I_{ij}|} \Big[\vec{\hat{F}}_{i+\frac{1}{2},j} - \vec{\hat{F}}_{i-\frac{1}{2},j} + \vec{\hat{G}}_{i,j+\frac{1}{2}} - \vec{\hat{G}}_{i,j-\frac{1}{2}} \Big],$$
(3)

where $|I_{ij}|$ is the area of the cell I_{ij} and $\overline{\vec{U}}_{ij}^n$ is the integral mean value of \vec{U} in the cell I_{ij} at time t^n . For constant matrices $\underline{\underline{A}}$ the flux F is given by

$$\vec{F}_{i+\frac{1}{2},j} = \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \underline{\underline{A}} \underbrace{\underline{1}}_{t^{n}} \int_{t^{n}}^{t^{n+1}} \vec{U} \left(x_{i+\frac{1}{2}}, \eta, \tau \right) \mathrm{d}\tau \,\mathrm{d}\eta = \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \underline{\underline{A}} \vec{U}^{\mathrm{ADER}} \left(x_{i+\frac{1}{2}}, \eta \right) \mathrm{d}\eta \tag{4}$$

with the integral mean value being solved by the ADER approach [7–9]

$$\vec{U}^{\text{ADER}} \equiv \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} \vec{U}(\vec{X}_0, t) dt = \sum_{k=0}^{\infty} \frac{(-\Delta t)^k}{(k+1)!} (\underline{\underline{A}}\partial_x + \underline{\underline{B}}\partial_y)^k \vec{U}(\vec{X}_0, t^n).$$
(5)

In the ADER approach the state $\vec{U}(\vec{X}_0, t)$ is calculated by a Taylor series. The time derivatives are then replaced by spatial derivatives with the Lax–Wendroff (or Cauchy–Kovalevskaja) procedure and is then integrated exactly.

For the construction of numerical schemes, the infinite sum in (5) cut off after (m-1) addends which leads to a scheme with order m in time.

Using a Gaussian quadrature formula, the space integral in (4) can be approximated by

$$\vec{F}_{i+\frac{1}{2},j} = \frac{\Delta y}{2} \sum_{\lambda=1}^{N_{\rm G}} \omega_{\lambda} \underline{\underline{\mathcal{A}}} \vec{U}^{\rm ADER}(x_{i+\frac{1}{2}}, \eta_{\lambda}), \tag{6}$$

where the ω_{λ} denote the weights of the quadrature, $N_{\rm G}$ is the total number and η_{λ} are the positions of the Gaussian quadrature points. It can be shown [11] that this approach is *m*th order accurate in space and time if the reconstructions for the derivatives are *m*th order in space.

An important step in high-order approximation of the fluxes is the method by which one obtains a high-order pointwise representation of the solution $\vec{U}^{(0)}(x, y, t)$ and their derivatives $\vec{U}^{(k)}(x, y, t)$ from the given cell averages $\vec{U}(t)$. For this purpose we use the conservative Lagrangian interpolation as given in [3,4,9].

In practical computations it is essential that any new scheme is comparable concerning CPU time and memory to existing schemes, if a solution of given quality has to be calculated. For aeroacoustical calculations such a benchmark scheme is, e.g., the dispersion relation preserving (DRP) scheme of Tam [10]. The ADER scheme in the original formulation as given above is slower than this reference scheme. In the following some possibilities are shown to make the algorithm much more efficient, at least in the linear case, considered in this paper.

If the following conditions are fulfilled:

- I. Linear systems with constant Jacobians A and B.
- II. Constant mesh size in x- and y-direction.

III. Constant time step.¹

IV. Linear reconstruction algorithm in space.

most of the calculations can be executed in a preprocessor step. From now on, we will call the resulting algorithm fast-ADER scheme when we refer to the fast implementation of the ADER approach which is going to be derived under restrictions I–IV.

First condition IV is used. For the solution of the hyperbolic PDE (1) a finite volume discretization (3) is applied with the numerical fluxes given by (6).

Two cases for the reconstructions must be analyzed:

- I. Even order schemes. If we use central stencils, a linear reconstruction procedure of even order is obtained. In this special case we have $\vec{U}^+ = \vec{U}^-$ for the values at the cell interface.
- II. Odd order schemes. If we use slightly non-centered stencils for the reconstruction from the left and from the right, different values at the interface are produced from both sides. The general solution of the Riemann problem $\vec{U}^{RP} = RP(\vec{U}^+, \vec{U}^-)$ is a function of the Jacobians \underline{A} , \underline{B} only and thus known at the beginning of the computation.

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¹ This condition can easily be given up, if the coefficients are recalculated partially for every time step.

The procedure described in the following applies to the even order schemes. We note that for odd order schemes a similar procedure can be derived, which is slightly more complicated due to the incorporation of the Riemann-solver. The flux is now given by

$$\vec{\hat{F}}_{i+\frac{1}{2},j} = \frac{\Delta y}{2} \sum_{\lambda=1}^{N_{\rm G}} \omega_{\lambda} \underline{\underline{A}} \sum_{k=0}^{\mathcal{O}-1} \frac{\left(-\Delta t\right)^{k}}{(k+1)!} \left[\sum_{m=k}^{0} \underline{\underline{M}}(\underline{\underline{A}}, \underline{\underline{B}}, k, m) \left(\sum_{ii=-\mathcal{O}/2+1}^{\mathcal{O}/2} \sum_{jj=-\mathcal{O}/2}^{\mathcal{O}/2} C_{ii,jj}^{m,k-m} \vec{U}_{i+ii,j+jj} \right) \right]$$
(7)

with

$$\underline{\underline{M}} = \underline{\underline{M}}(\underline{\underline{A}}, \underline{\underline{B}}, k, m) = \sum_{I_{m,k}} \prod_{r=1}^{k} (\underline{\underline{A}}^{p_r} \cdot \underline{\underline{B}}^{q_r})$$
(8)

and

$$I_{m,k} := \left\{ ((p_r, q_r))_{r=1}^k : p_r, q_r \in \{0, 1\}, p_r + q_r = 1, \sum_{r=1}^k p_r = m, \sum_{r=1}^k q_r = k - m \right\}.$$
(9)

In the next step constant mesh sizes in x- and y-direction are assumed (condition II). Thus the coefficients $C_{i,j}^{n_x,n_y}$ are constant for every cell and the brackets of Eq. (7) can be re-ordered:

$$\vec{F}_{i+\frac{1}{2}j} = \sum_{ii=-\ell/2+1}^{\ell/2} \sum_{jj=-\ell/2}^{\ell/2} \left[\frac{\Delta y}{2} \sum_{\lambda=1}^{N_{\rm G}} \omega_{\lambda} \underline{\underline{\mathcal{A}}} \sum_{k=0}^{\ell-1} \frac{(-\Delta t)^k}{(k+1)!} \left(\sum_{m=k}^{0} \underline{\underline{\mathcal{M}}}(\underline{\underline{\mathcal{A}}}, \underline{\underline{B}}, k, m) C_{ii,jj}^{m,k-m} \right) \right] \vec{U}_{i+ii,j+jj} \tag{10}$$

$$=\sum_{ii=-\ell/2+1}^{\ell/2}\sum_{jj=-\ell/2}^{\ell/2}\underline{\underline{C}}_{ii,jj}^{*}\vec{U}_{i+ii,j+jj}.$$
(11)

The new constant $\underline{C}_{[i,j]}^*$ is now a $n \times n$ matrix instead of a scalar, with *n* being the dimension of the state vector \vec{U} . This new constant contains all information about the Jacobians of the system, the Gaussian integration for the high order flux calculation and the high order reconstruction of the derivatives.

In a last step, the finite volume scheme (3) is given with the discrete fluxes (11) as

$$\overline{\vec{U}}_{ij}^{n+1} = \overline{\vec{U}}_{ij}^{n} - \left[\sum_{ii=-\ell/2}^{\ell/2} \sum_{jj=-\ell/2}^{\ell/2} \underline{\underline{C}}_{ii,jj}^{**} \vec{U}_{i+ii,j+jj}\right].$$
(12)

The coefficient matrix $\underline{\underline{C}}_{ii,jj}^{**}$ is a combination of $\underline{\underline{C}}^{X*}$ and $\underline{\underline{C}}^{Y*}$ multiplied by $\Delta t/|I_{ij}|$. If the Jacobians $\underline{\underline{A}}$ and $\underline{\underline{B}}$ are constant in the domain (condition I.), the constant $\underline{\underline{C}}^{**}$ can be used for every cell.

We note that scheme (12) now has the structure of a single-step finite difference scheme but with a real two-dimensional stencil, which does spatial and temporal discretization at the same time. It is obvious, that the ADER approach in this fast formulation needs less memory than a finite difference discretization with the same spatial order and Runge–Kutta time discretization.

Note on the 2nd order scheme. For the second order scheme two Gaussian integration points in (6) or (10) must be used for stability reasons. The resulting scheme is identical to the one-step Lax–Wendroff scheme in two dimensions, described by Hirsch [6] in equation (17.2.48).

The computational effort of the scheme can be estimated easily. The number of points included in the stencil grows quadratically with the order $((k + 1) \times (k + 1)$ points). As the scheme is always one single step in time, the CPU effort grows also quadratically. This is illustrated in Fig. 1, obtained by measuring the CPU time for a given example. The estimated values are in good agreement with the predicted values. The

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Fig. 1. CPU effort depending on the order of the scheme, normalized to the second order scheme.

growth rate is a little bit lower which may be due to a better use of the CPU cache for higher order schemes. For comparison the DRP scheme of Tam [10] has been added to the graph. It is a formally fourth order scheme in space, which is derived from a sixth order finite-difference scheme. For the integration in time a standard fourth order Runge-Kutta scheme has been used. We note that the order of accuracy in our test calculations was limited to the 24th order. This was due to the facts that the accuracy needed for the computation of the coefficients in (12) was not sufficient even using double precision variables. The reduction of the computational effort with respect to the original formulation is significant: For a 10th order scheme the factor is ≈ 300 and for the 20th order scheme it is ≈ 2000 .

3. Numerical results

In Computational AeroAcoustics (CAA) good wave propagation properties are a crucial point for numerical schemes. The dispersion and dissipation errors must be as low as possible in order to provide accurate wave propagation over long distances on reasonably coarse grids. In [7,9] we plotted the amplitude- and phase errors for the ADER approach. As nothing is neglected, they apply without any change to the fast-ADER approach. An $\mathcal{O}4$ ADER scheme has approximately the same phase error as a sixth order standard finite difference scheme. The amplitude errors do not depend very much on spatial discretization but on the time discretization, so that the amplitude errors for all schemes which are fourth order in time are quite similar. However with the ADER approach it is easy to obtain even higher order time discretizations which leads to considerably lower amplitude errors.

Next, we show numerical convergence studies for a two-dimensional test case for the linearized Euler equations

$$\vec{U}_t + \underline{\underline{A}}_0 \ \vec{U}_x + \underline{\underline{B}}_0 \ \vec{U}_y = 0 \tag{13}$$

with

$$ec{U} = egin{pmatrix}
ho' \ u' \ v' \ p' \end{pmatrix}, \quad A_0 = egin{pmatrix} u_0 &
ho_0 & 0 & 0 \ 0 & u_0 & 0 & rac{1}{
ho_0} \ 0 & 0 & u_0 & 0 \ 0 & \gamma p_0 & 0 & u_0 \end{pmatrix}, \quad B_0 = egin{pmatrix} v_0 & 0 &
ho_0 & 0 \ 0 & v_0 & 0 & 0 \ 0 & 0 & v_0 & rac{1}{
ho_0} \ 0 & 0 & \gamma p_0 & v_0 \end{pmatrix}.$$

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The values to compute the (space-time constant) matrices $\underline{\underline{A}}_0$ and $\underline{\underline{B}}_0$ are $\rho_0 = 1$, $u_0 = 1$, $v_0 = 1$ and $p_0 = \rho_0/\gamma$ with $\gamma = 1.4$. The setup is an initial Gaussian density pulse of the form

$$\rho'(x, y, t = 0) = e^{-(1/2)(x^2 + y^2/\sigma^2)}$$
(14)

with halfwidth σ which is advected through the computational domain along the diagonal y = x. The other variables u', v' and p' are initialized with 0. The computational domain has the extents $[100 \times 100]$ units, the boundary conditions are periodic and the error with respect to the exact solution is calculated after one period of advection (T = 100). The CFL number is set to v = 0.67 and the number of gridpoints in x and y direction is N_G . A three dimensional plot of the solution after 100 periods is given in Fig. 2 for the DRP scheme of Tam [10] with Runge–Kutta fourth order time integration and for the ADER schemes of order $\mathcal{O}4 - 12$. Table 1 show clearly that the respective design orders of the numerical schemes have been reached well for the $\mathcal{O}6$ scheme. If we go to higher order schemes ($\mathcal{O}16$), we get the problem that the resolution of the scheme reaches machine precision for all wavelengths that can be resolved on a given grid. With mesh refinement, the design order can not completely be retrieved for a given problem because of the limited machine precision. Thus a sharper Gauss pulse $\sigma = 2$ units is used for the ADER $\mathcal{O}16$ in order to increase the errors and in order to avoid reaching machine precision too fast. Though being below the design order of 16, the numerical convergence rate nevertheless confirms that the construction of very high order schemes with the ADER approach is possible and that the only limiting factors are the resolution of the grid and machine precision.



Fig. 2. Gausspuls with halfwidth of $\sigma = 3$ units at $T_{end} = 10,000$, $T_{end}^{DRP} = 12,000\Delta t$, $T_{end}^{ADER} = 15,000\Delta t$. ($\Delta x = \Delta y = 1$, $u_0 = v_0 = 1$). (a) DRP- $\mathcal{O}4/RK-\mathcal{O}4$, (b) ADER $\mathcal{O}4$, (c) ADER $\mathcal{O}6$, (d) ADER $\mathcal{O}12$.

N _G	ADER $\emptyset 6, \sigma = 3$		ADER $\emptyset 16, \sigma = 2$		
	L_1	\mathcal{O}_{L_1}	$\overline{L_1}$	\mathcal{O}_{L_1}	
75×75	2.6687E-04		7.6325E-05		
100×100	3.6913E-05	6.9	3.9629E - 06	10.3	
150×150	3.4632E - 06	5.8	2.0751E - 08	13.0	
200×200	6.2457E-07	6.0	3.1870E - 10	14.5	
300×300	5.6160E - 08	5.9	6.7906E - 13	15.2	
400 imes 400	9.9998E - 09	6.0	8.1115E – 15	15.4	

Table 1 Numerical convergence rate for ADER 06/016 scheme

4. Conclusions

If the following assumptions hold: The mesh sizes Δx and Δy is constant and the PDE is linear with constant coefficients, then the fast formulation of the ADER scheme leads to a single-step scheme in time of arbitrary order of accuracy which is dramatically faster than the original formulation. For the 20th order scheme the speed-up is about 2000. We implemented the scheme in such a way, that the order of accuracy in space and time becomes only a parameter to be specified, so a really arbitrary high order implementation of ADER schemes has been achieved. The practical limit is given only by computer precision in the calculation of the coefficients. Compared to other high-order integration schemes in time such as Runge-Kutta methods this is a clear benefit, because Runge-Kutta methods suffer from the Butcher barriers for orders higher than four. The fast-ADER scheme has a very compact computational kernel which can be optimized very efficiently. In one and two dimensions the second order scheme is identical to the classical second order one-step Lax-Wendroff scheme. The ADER scheme was compared to standard finite difference schemes, using Runge-Kutta time integration. Finally we presented a numerical convergence study for the two dimensional schemes up to O16. For very high order schemes the accuracy of practical computations is limited by machine precision, as seen, e.g., in Table 1. The computational effort grows quadratically with the order of accuracy of the fast-ADER scheme due to the quadratic growth of the stencil size. The schemes presented in this paper are based on *linear* central reconstructions and are designed to capture linear wave propagation with small dissipation and dispersion errors. Thus it is clear, that they cannot be TVD. If discontinuities were inherent in the solution, other reconstruction techniques like WENO should be used. The extension to three dimensions is straight forward. Further work on ADER schemes has to be done for nonlinear systems and for reconstruction on unstructured meshes.

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