In: Proceedings of the 11th Finnish Mechanics Days. (2012)

Optimized low-order explicit Runge-Kutta schemes for the high-order spectral difference method

Matteo Parsani, David I. Ketcheson and Willem Deconinck

Summary. Optimal explicit Runge-Kutta (ERK) schemes with large stable step sizes are developed for method-of-lines discretizations based on the spectral difference (SD) spatial discretization on quadrilateral grids. These methods involve many stages and provide the optimal linearly stable time step for a prescribed SD spectrum and the minimum leading truncation error coefficient, while admitting a low-storage implementation. Using a large number of stages, the new ERK schemes lead to efficiency improvements larger than 60% over standard ERK schemes for 4^{th}- and 5^{th}-order spatial discretization.

Key words: Optimized explicit Runge-Kutta, High-order spectral difference method, Wave propagation.

Introduction

Throughout the past two decades, the development of high-order accurate spatial discretization has been one of the major fields of research in computational fluid dynamics (CFD), computational aeroacoustics (CAA), computational electromagnetism (CEM) and in general computational physics. High-order discretizations have the potential to improve the computational efficiency required to achieve a desired error level by allowing use of coarser grids. Moreover, since computational science is increasingly used as an industrial design and analysis tool, high-order accuracy must be achieved on unstructured grids, which are required for efficient meshing. These needs have been the driving force for the development of a variety of higher order schemes for unstructured meshes such as the Discontinuous Galerkin (DG) method [1], the Spectral Volume (SV) method [2], the Spectral Difference (SD) method [3], the Energy Stable Flux Reconstruction [4], etc.

High-order schemes are usually much stiffer than lower-order ones, so the maximum stable CFL number usually decreases rapidly with increasing order of accuracy. Therefore, the step size is often based on stability considerations when obtaining time-accurate solutions with explicit schemes.

This work focuses on the development of new optimized ERK schemes for accurate and efficient computation of wave propagation problems with high-order SD methods. A two-step optimization procedure is used to design optimal ERK schemes. First, a new, robust, fast and accurate optimization algorithm is employed to find the optimal stability function that maximizes the linear stable step size of the ERK scheme for a prescribed SD Fourier footprint computed by discretizing the two-dimensional (2D) advection equation. A second optimization step is used to determine the Butcher coefficients of the scheme, optimized for a small leading truncation error constant and constrained to be implementable in a low-storage form.

In [5] has been shown that the SD discretization error typically dominates, when both spatial and temporal discretizations have the same accuracy. Therefore, for a fixed order

of accuracy the error is almost independent of the CFL number and large time steps can be used. This feature has led to a new ongoing line of research where the ultimate goal is to investigated if efficient and accurate low-order ERK schemes can be developed for high-order SD discretizations. In fact, the coefficients of a low-order method must satisfy fewer order conditions which implies a larger number of free parameters in the optimization process. Following this idea, we present the performance of low-order ERK schemes for a 4^{th}-order SD discretization applied to a compressible Euler flow past a wedge.

Spectral difference method

Consider a problem governed by a general system of conservation laws given by Equation (1) and valid on a domain $\Omega \subset \mathbb{R}^d$ and completed with consistent initial and boundary conditions.

$$\frac{\partial \mathbf{w}}{\partial t} + \vec{\nabla} \cdot \vec{\mathbf{f}} = 0, \tag{1}$$

The domain is divided into N non-overlapping cells. In order to achieve an efficient implementation of the SD method, all hexahedral cells in the physical domain are mapped into cubic elements using local coordinates $\vec{\xi} = [\xi_1, \xi_2, \xi_3]^T$. Such a transformation is characterized by the Jacobian matrix $\vec{\vec{\mathrm{J}}}_i$ with determinant $det(\vec{\vec{\mathrm{J}}}_i)$. Therefore, system (1) can be written in the mapped coordinate system as

$$\frac{\partial \mathbf{w}_i^{\vec{\xi}}}{\partial t} = -\frac{\partial \mathbf{f}_{1,i}^{\vec{\xi}}}{\partial \xi_1} - \frac{\partial \mathbf{f}_{2,i}^{\vec{\xi}}}{\partial \xi_2} - \frac{\partial \mathbf{f}_{3,i}^{\vec{\xi}}}{\partial \xi_3} = -\vec{\nabla}^{\vec{\xi}} \cdot \vec{\mathbf{f}}_i^{\vec{\xi}}, \qquad 1 \leq i \leq N, \tag{2}$$

where $\mathbf{w}_i^{\vec{\xi}} \equiv det(\vec{\vec{\mathrm{J}}}_i)\,\mathbf{w}$ and $\vec{\nabla}^{\vec{\xi}}$ are the conserved variables and the divergence differential operator in the mapped coordinate system, respectively.

For a $(p+1)$-th-order accurate d-dimensional scheme, N^s *solution collocation points* with index j are introduced at positions $\vec{\xi}_j^s$ in each cell i, with N^s given by $N^s = (p+1)^d$. Given the values at these points, a polynomial approximation of degree p of the solution in cell i can be constructed. This polynomial is called the *solution polynomial* and is usually composed of a set of Lagrangian basis polynomial $L_j^s\left(\vec{\xi}\right)$ of degree p:

$$\mathbf{W}_i\left(\vec{\xi}\right) = \sum_{j=1}^{N^s} \mathbf{W}_{i,j}\, L_j^s\left(\vec{\xi}\right), \qquad 1 \leq i \leq N. \tag{3}$$

The interpolation coefficients $\mathbf{W}_{i,j}$ are the unknowns of the SD method.

The divergence of the mapped fluxes $\vec{\nabla}^{\vec{\xi}} \cdot \vec{\mathbf{f}}^{\vec{\xi}}$ at the solution points is computed by introducing a set of N^f flux collocation points with index l and at positions $\vec{\xi}_l^f$, supporting a polynomial of degree $p+1$. The evolution of the mapped flux vector $\vec{\mathbf{f}}^{\vec{\xi}}$ in cell i is then approximated by a flux polynomial $\vec{\mathbf{F}}_i^{\vec{\xi}}$, which is obtained by reconstructing the solution variables at the flux points and evaluating the fluxes $\vec{\mathbf{F}}_{i,l}^{\vec{\xi}}$ at these points. The flux is also represented by a Lagrange polynomial:

$$\vec{\mathbf{F}}_i^{\vec{\xi}}\left(\vec{\xi}\right) = \sum_{l=1}^{N^f} \vec{\mathbf{F}}_{i,l}^{\vec{\xi}}\, L_l^f\left(\vec{\xi}\right), \tag{4}$$

The solution at a face is in general not continuous and requires the solution of a Riemann problem to maintain conservation at a cell level. Approximate Riemann solvers, such as the Roe solver, are typically used. The tangential component of $\vec{\mathbf{F}}^{\vec{\xi}}_{\text{num}}$ is usually taken from the interior cell.

Taking the divergence of the flux polynomial $\vec{\nabla}^{\vec{\xi}} \cdot \vec{\mathbf{F}}^{\vec{\xi}}_i$ in the solution points results in the following modified form of (2):

$$\frac{d\mathbf{W}_{i,j}}{dt} = -\vec{\nabla} \cdot \vec{\mathbf{F}}_i \Big|_j = -\frac{1}{J_{i,j}} \vec{\nabla}^{\vec{\xi}} \cdot \vec{\mathbf{F}}^{\vec{\xi}}_i \Big|_j = \mathbf{R}_{i,j}, \tag{5}$$

where $\mathbf{R}_{i,j}$ is the SD residual associated with $\mathbf{W}_{i,j}$. This is a system of ODEs, in time, for the unknowns $\mathbf{W}_{i,j}$ which will be solved with the new optimized ERK schemes presented in this work.

Optimized Runge–Kutta schemes

In general, the stability function $\psi(z)$ for an s-stage, order p, ERK method is a polynomial of degree s that differs from the exponential function by terms of order z^{p+1}:

$$\psi(z) = \sum_{j=0}^{s} \beta_j z^j = \sum_{j=0}^{p} \frac{1}{j!} z^j + \sum_{j=p+1}^{s} \beta_j z^j, \tag{6}$$

where z is in general a complex number.

It is natural then to design optimal polynomials by choosing the coefficients β_j in (6) so as to maximize maximum linearly stable CFL number ν_{stab}. The optimization problem may be stated formally as follows

Problem 1 (Stability polynomial optimization)

$$\begin{aligned} &\textit{maximize} \quad \nu \\ &\text{subject to} \\ &\qquad |\psi(\nu\lambda)| \leq 1 \quad \textit{for all } \lambda \in \sigma(\mathbf{L}) \\ &\qquad \psi(z) - \exp(z) = \mathcal{O}(z^{p+1}). \end{aligned}$$

We solve Problem 1 using a convex optimization approach and bisection with respect to the CFL number ν, as described in [6]. This approach allows us to optimize methods with large numbers of stages in order to improve the maximum absolutely stable time step ν_{stab}. The optimization is carried out for 2^{nd}- to 5^{th}-order accurate schemes; the constraint points λ are taken as the spectrum of the SD semi-discretization of the 2D advection equation [5].

The choice of stability polynomial does not fully determine the method; an ERK method of s stages has $s(s+1)/2$ coefficients and only s of them are constrained by the stability polynomial. We use the remaining degrees of freedom to satisfy additional nonlinear order conditions ($\tau_i^{(j)}(\mathbf{A}, \mathbf{b}) = 0$), to obtain a low-storage implementation, and ensure that the truncation error coefficients $C^{(p+1)}$ is not too large. This leads to the computation of the so called Butcher's coefficients $\mathbf{A}, \mathbf{b}$. The optimization problem may be stated formally as follows:

Method	s	ν_{stab}/s	$C^{(p+1)}$
Kutta's ERK(4,4)	*4*	3.9534×10^{-02}	1.4505×10^{-02}
Optimal ERK(9,4) [5]	9	5.6977×10^{-02}	5.0640×10^{-04}
Optimal ERK(18,4) [5]	18	6.5233×10^{-02}	1.1087×10^{-04}
Optimal ERK(4,1)	4	6.6877×10^{-02}	1.6427×10^{-02}
Optimal ERK(9,1)	4	6.8593×10^{-02}	3.9650×10^{-04}
Optimal ERK(18,1)	18	6.8832×10^{-02}	4.1898×10^{-08}

Table 1. Effective step size and leading truncation error coefficient of the optimal ERK methods used in this work. The 4-stage method (corresponding to the values in italics) is the classic ERK method.

Problem 2 (RK method optimization)

$$
\begin{aligned}
&\textit{minimize} \quad C^{(p+1)} \\
&\text{subject to} \\
&\qquad \tau_i^{(j)}(\mathbf{A},\mathbf{b}) = 0 \quad (0 \le j \le p) \\
&\qquad \mathbf{b}^T\mathbf{A}^{j-1}\mathbf{e} = \beta_j \quad (0 \le j \le s) \\
&\qquad \Gamma(\mathbf{A},\mathbf{b}) = 0
\end{aligned}
$$

Here $\mathbf{b}^T\mathbf{A}^{j-1}\mathbf{e} = \beta_j$ and $\Gamma(\mathbf{A},\mathbf{b}) = 0$ represent the prescribed stability polynomial coefficients β_j and the conditions necessary for the method to be written in low-storage form [7], respectively.

We have computed optimized methods for $s \le 20$, because for larger values of s, the convex solvers used in the algorithm of [6] often fail due to poor numerical conditioning. The order of accuracy of the SD scheme has been fixed to four ($p = 3$) whereas the order of accuracy of the optimized ERK schemes has been varied from one to three (i.e. $p-1$). In this work we show present three new 1$^{\text{st}}$-order accurate optimized ERK schemes with respectively 4, 9 and 18 stages (i.e., ERK(4,1), ERK(9,1) and ERK(18,1)) and we compare their performance with the optimized 4$^{\text{tt}}$-order methods with the same number of stages recently presented in [5].

Table 1 lists the value of the effective time step and the leading truncation error coefficient of the optimized ERK schemes used for the test problem in the next section.

Flow past a wedge

In this section, the compressible Euler flow past a triangular wedge is discretized using a highly unstructured mesh and is used to study the performance of two new 1$^{\text{st}}$-order ERK schemes. In Figure 1 the density contour at $t = 200$ is shown, where the incoming flow is from left to right. The wedge is placed on the centerline $y = 0$ of the computational domain and it is characterized by a length L. At the left boundary (the inflow) the flow is prescribed to be uniform with zero angle of attack and free-stream Mach number of 0.2. Both inlet density and inlet pressure are set to one. A pressure outlet boundary condition is imposed on the right boundary of the domain which is placed about 20 L away from the wedge. Far-field boundary conditions (i.e. uniform Dirichlet boundary conditions for the conserved variables) are imposed both on the top and bottom boundaries.

An unstructured grid with $2,952$ quadrilateral cells with a maximum aspect ratio of 1.6 is used. The total number of DOFs is $47,232$. Several computations are performed using the CFL number ν_{stab} for each scheme and measuring the error after 0.1 seconds.

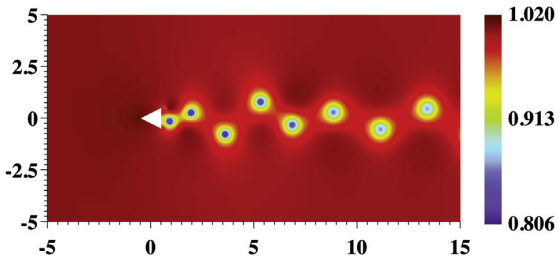
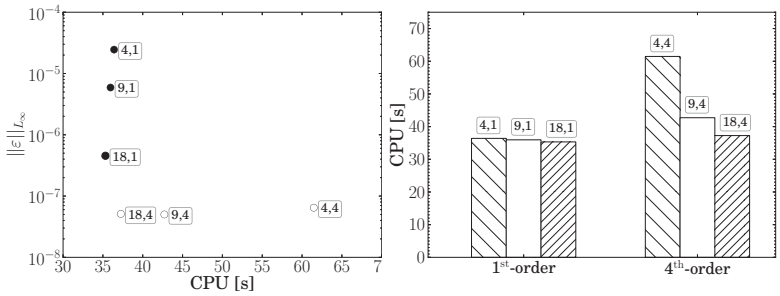


Figure 1. Density contour of the flow past a wedge at $t = 200$.

A reference solution is numerically computed by solving the problem on the mesh with $11,686$ quadrilateral cells with the 5^{th}-order SD method ($292,150$ DOFs) and the explicit 6-stage 5^{th}-order Runge–Kutta–Fehlberg (ERKF(6,5)) scheme. A CFL number $\nu = 0.1$ is used for the reference computation.

Starting with an already developed solution, several computations are performed using the CFL number ν_{stab} for each scheme and measuring the error after 0.1 seconds. Figure 2 shows the maximum norm of the error and the CPU time for the classical 4-stage 4^{th}-order ERK(4,4) scheme, the 4^{th}-order optimized methods presented in [5] and the new 1^{st}-order time stepping.

Remarkably, we observe that the new schemes, designed using linear advection on a uniform grid, perform very well also for the compressible Euler equations on an unstructured quasi-uniform grid.



(a) Error versus CPU time. (b) CPU time for each simulation.

Figure 2. Error and CPU time for the wedge problem. The labels s, p for each point indicate the number of stages s and the order p of the corresponding scheme. Open circles are used for the reference methods.

By using a lower order of accuracy we have been able to increase the linearly stable step size of the solver by about 60% and 17%, respectively, over the standard ERK(4,4) scheme and the ERK(9,4) method presented in [5]. However, for the 18 stage method the gain is about 5%. Such improvements are obtained with some sacrifices in accuracy, though the global error obtained by using the ERK(18,1) method is still small.

Conclusions and future directions

In this work the performance of new optimized first-order ERK schemes for the high-order spectral difference method on unstructured quasi-uniform tensorial cell grids have

been presented. A comparison with the recently proposed optimized 4^{th}-order schemes reported in [5] has also been reported. We have observed that if a small or a medium number of stages is used and an integration error of about $10^{-4} - 10^{-5}$ is acceptable the low-order accurate ERK schemes represent a valid alternative to the standard high-order methods when simulations running on expensive supercomputers for hundreds of hours must be integrated as fast as possible.

The optimization of low-order ERK schemes for the SD methods is still an ongoing research and will be completed in the near future with the development of ERK schemes with embedded error estimators.

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Matteo Parsani, David I. Ketcheson
King Abdullah University of Science and Technology
Division of Mathematical and Computer Sciences and Engineering
23955-6900 Thuwal, Saudi Arabia
matteo.parsani@kaust.edu.sa, david.ketcheson@kaust.edu.sa

Willem Deconinck
Vrije Universiteit Brussel
Department of Mechanical Engineering
Pleinlaan 2, 1050 Brussels. Belgium
willem.deconinck@vub.ac.be