Comparison of Traditional and Novel Discretization Methods for Advection Models in Numerical Weather Prediction

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Abstract. Numerical Weather Prediction has been dominated by low order finite difference methodology over many years. The advent of high performance computers and the development of high order methods over the last two decades point to a need to investigate the use of more advanced numerical techniques in this field. Domain decomposable high order methods such as spectral element and discontinuous Galerkin, while generally more expensive (except perhaps in the context of high performance computing), exhibit faster convergence to high accuracy solutions and can locally resolve highly nonlinear phenomena. This paper presents comparisons of CPU time, number of degrees of freedom and overall behavior of solutions for finite difference, spectral difference and discontinuous Galerkin methods on two model advection problems. In particular, spectral differencing is investigated as an alternative to spectral-based methods which exhibit stringent explicit time step requirements.

Keywords: Numerical weather prediction, spectral differencing, discontinuous Galerkin, advection.

1 Introduction

The science of meteorology relies heavily on numerical simulations of the equations that govern the atmosphere. These computations combine observational data and scientific theory to enhance understanding of complex meteorological phenomena. The aim of Numerical Weather Prediction (NWP) is to diagnose the state of the atmosphere and rapidly deliver a prognosis for its future state. Hence the importance of using highly accurate as well as efficient numerical techniques cannot be overstated. While it is true that the current challenges in NWP are associated with parameterization of sub-grid scale processes, whose cost eclipses that of the underlying dynamics, parameterization accuracy in NWP applications depends on the accurate transport of the Reynolds averaged variables to the correct locations at the correct time with the correct structure. Optimizing the accuracy by using higher order schemes involving fewer degrees of freedom can engender significant cost savings in the calculation of these many physical processes.

Finite difference (FD) numerical methods have been very successful in meteorological modeling. They are easily formulated, well documented and studied, and foster an intuitive computer programming implementation. These methods are intrinsic components of most of today's state-of-the-art dynamical cores in research and operational models. Simply put, they are efficient, comfortable, and proven.

Classic spectral numerical methods have been used in the direct numerical simulation of turbulence and in the arena of global climate modeling. These methods provide exponential convergence, low diffusive and dispersive errors, and have been proven to be more efficient than FD methods when high accuracy or long time integration is required [1]. These methods, however, have not been used extensively in NWP, for which computational efficiency is arguably as important as accuracy. For the same computation, spectral methods require more operations, and often impose more severe time step restrictions, than FD methods. The global property of these methods, which enables their high accuracy, can also destroy their ability to be decomposed in parallel computing architectures.

Element-based spectral (EBS) methods, developed in the last 25 years, are a relatively new approach to numerical modeling. These methods feature the desired localization of FD stencils, as a domain is discretized into smaller sub-domains, or elements, in which local approximations are made. They also provide the formal accuracy and wave propagation properties of classic spectral methods. Of potentially greater importance, EBS methods provide the seemingly ideal framework to exploit high performance computing architectures of the present and future. While these methods are promising, and have been used extensively in engineering, they remain relatively unexplored in NWP, although several on-going efforts, *e.g.* [2,3,4], in global (climate) atmospheric science have proven them worthy of pursuit.

Our work seeks to quantify the differences between FD and EBS methods in terms of accuracy and computational efficiency. The intent is not necessarily to prove one method superior to another, but rather to elucidate the strengths, weaknesses, and behaviors of the methods in modeling meteorological phenomena. It is hoped that a greater understanding of EBS methods will help identify their potential use in meteorological codes. This paper will focus on the introduction of the spectral differencing method as an alternative to FD and Galerkin-based EBS methods.

2 Discretization Methods

With the promise of higher accuracy and potentially corresponding high efficiency, we investigate EBS methods for simple NWP advection models. High order EBS methods rely on spectral decomposition of the solution on sub-domains or elements in terms of high order orthogonal polynomials with corresponding high order quadrature-rule points. The distribution of these points is non-equal in space, necessitating stricter time step requirements in explicit schemes. This single issue has damped the enthusiasm of NWP investigators to consider high order methods. Spectral elements (SE) and discontinuous Galerkin (DG) are two such methods that show promise for NWP. However, the global continuity and the only globally conservative feature of SE also present drawbacks for NWP. DG, on the other hand, provides local conservation and greater flexibility for parallel computing through the calculation of fluxes at element interfaces. Spectral differencing (SD) presents itself as a perhaps viable

alternative to all of these methods: it combines the high order advantages of EBS methods with the collocation approach of FD methods. Furthermore, through recent work, it has been found that the choice of the collocation points can be changed with only slight effect on accuracy, thereby alleviating the restrictions of small time steps. We present here a short description of the SD method and provide a stability analysis.

2.1 Spectral Differencing

The spectral difference method (SD) was first proposed by Kopriva and Kolas [5] under the name “conservative staggered-grid Chebyshev multidomain method.” The authors used the method to solve the Euler equations for a number of compressible flows, for varying geometries. Like DG, SD was developed, in part, as a way to discretize and solve problems involving complex geometries. Similar to FD, the staggered grid was constructed to ensure conservation and remove the solution points from boundaries, thus alleviating problems with sub-domain corners and boundary conditions. See the grid in Fig. 1a. The name “spectral difference” was coined by Liu *et al.* [6], who reprised a slight variance on the original Chebyshev multi-domain method. SD was sought after as an alternative to spectral methods that require quadrature.

Van den Abeele *et al.* [7], recently provided an analysis of the stability of SD, and found that the method can be unstable under certain conditions. The method to stabilize the scheme proposed in [7] is to “cluster” the interior flux points toward the element edges in a manner proven to eliminate the positive real Fourier footprint of the spatial discretization, as shown in Fig. 1b). This paper also showed that the numerical dispersion relation is independent of the position of the solution points, which means that the solution points can be placed arbitrarily without affecting the stability or dispersive properties of the method. This leads to an important gain in the efficiency of the method. The solution points can be placed at flux points thereby reducing the amount of interpolation required when the solution polynomial is interpolated to the flux grid. When a solution point is collocated with a flux point, no interpolation to

Fig. 1. The spectral difference collocation staggered grids of a) Kopriva and Kolas [5] b) Van den Abeele *et al.* [7] and c) the present study for an 8th order approximation. The red circles represent the grid on which the solution is defined over one element. The blue squares represent the grid on which the flux is computed. The red circles overlaid on blue squares represent flux points at which solution points have been placed.

that flux point is needed; the value of the solution is simply transferred to the flux point. If the solution points are to remain off the element boundaries, one of the desirable properties of the staggered grid, then they are only overlaid at interior flux points. The SD formulation used in this study is a combination of the original method of Kopriva and Kalias [5] and the new method of Van den Abeele *et al.* [7]. The Gauss Lobatto Chebyshev quadrature nodes are used as the flux points, as in [5], but the solution point independence demonstrated by [7] is exploited as shown in Fig. 1c). Thus, both the severe time step restriction of the “stretched” flux points of [7], and the need to interpolate the solution polynomial to all flux points as in [5], are avoided.

The stability analysis is a variance on the traditional von Neumann wave analysis for linear problems. The von Neumann method represents the discretized solution at time n by a finite Fourier series,

$$\phi_j^n = \sum_{k=-N}^N a_k^n \exp(ikj\Delta x), \quad (1)$$

and examines the stability of an arbitrary Fourier mode, $\exp(ikj\Delta x)$. Finite Fourier series have the property that individual modes are eigenfunctions of linear FD operators [8] so the solution at time $n+1$ can be represented as

$$\phi_j^{n+1} = A_k \exp(ikj\Delta x), \quad (2)$$

where A_k is a complex constant known as the “amplification factor.” The amplification factor does not vary from time step to time step, so the stability of each Fourier mode is determined by the modulus of its amplification factor. The von Neumann stability condition

$$|A_k| \leq 1, \quad (3)$$

ensures that all resolvable Fourier modes are stable. The solution, Eqn. (1), will then be guaranteed to be stable since it is a linear combination of Fourier modes. The present stability analysis for the one-dimensional linear advection equation, similar to that of [7], represents the operators involved in a SD time step by a single matrix. If the vector of solution values at time n is u , then solution at time $n+1$ is

$$u^{n+1} = Bu^n, \quad (4)$$

where B is the operator matrix constructed by the SD interpolation, flux differentiation, and 3rd order Runge-Kutta time integration. Van den Abeele *et al.* [7] determined that for linear problems, an upwind flux is unstable for approximation order two and higher when the Gauss Lobatto Chebyshev quadrature nodes are used as the flux points. This analysis was performed for the SD spatial discretization and an Euler forward step in time. The present analysis, though for a 3rd order Runge-Kutta time integration, verifies these findings. Fig. 2 shows plots of the maximum eigenvalue versus the Courant number, $c\Delta t/\Delta x$, for $N = 4, 8$ approximations using a Lax-Friedrichs (corresponding to upwind in this case) flux. Within the range of reasonable Courant numbers, both plots clearly show an area for which the maximum eigenvalue exceeds one, and is therefore unstable. Note that, for a given order of approximation, not all Courant numbers are unstable. The range of unstable Courant numbers decreases with increasing order of approximation, as does the magnitude of the maximum eigenvalues. The 8th order

instability is particularly small. Using a sine wave initial condition, a wave speed of unity, 10 elements, and a Courant number of 0.1, the 8th order SD approximation took approximately 12,700,000 time steps before the solution demonstrated instability!

Fig. 2. Maximum eigenvalue of the amplification matrix of the spectral differencing operator with Lax-Friedrichs flux calculation as a function of Courant number for 4th (left) and 8th (right) order basis polynomials. Notice the difference in scale.

Van den Abeele *et al.* [7] did not address the use of any other numerical flux for linear problems, perhaps for good reason. The upwind flux for linear problems makes the most sense physically. When all waves travel with the same speed and in the same direction, all information is being propagated from only the upwind direction.

Nonetheless, in order to fully evaluate SD, we consider a central flux for the one-dimensional linear advection equation using the Gauss Lobatto Chebyshev flux points. It is found that the central flux is stable: for all orders of approximation investigated ($N = 2, \dots, 10$), the maximum eigenvalue never exceeds one within the range of reasonable Courant numbers. In particular, for $N=4$, the method is stable for Courant numbers < 1.096 , and, for $N=8$, for Courant < 0.605 . As with FD schemes, the maximum stable Courant number decreases with increasing order of approximation, but asymptotes in the vicinity of 8th order schemes. Both central and Lax-Friedrichs (L-F) fluxes were investigated in the numerical tests. More details on the stability analysis are available in Williams' thesis [9].

With these stability and time step restrictions in mind, a new SD grid is adopted that places the flux points at the Gauss Lobatto Chebyshev quadrature nodes and overlays the solution points on flux points, as was suggested by [7]. Fig. 1c) shows the grid for 8th order approximations. The new SD grid (Fig. 1c)) is much more regularly spaced than that of [7] especially for orders of 6 and higher. The time step restriction for the new SD grid is greatly reduced from that imposed by the grid in [7].

2.2 Finite Differencing

The SD method will be compared with standard finite differencing (see Durran [8] for example) of orders 2, 4, and 6, since these are the most commonly used NWP FD stencils. The equations will be solved in flux form to match the DG and SD formulations

and because the flux form is useful to ensure conservation in NWP. The spatial derivatives are computed for the fluxes, which are functions of the vector solution values. The staggered grid interpolation of Shchepetkin and McWilliams [10] is employed. Details are given in [9].

2.3 Discontinuous Galerkin Method

The DG method is a weighted residual technique requiring flux corrections at discontinuous element interfaces as a result of integration by parts of the weak form to ensure conservation. The present implementation follows derivations of Cockburn and Shu [11] with Lax-Friedrichs flux calculation. Legendre polynomial basis functions are used along with Gauss Lobatto Legendre quadrature. Details are given in [9]. Numerical results for DG, SD and FD discretizations are compared in the next section.

3 Numerical Tests

In order to verify the stability results of the preceding sections and to examine other properties of the schemes, such as dissipation and dispersion, several test problems were solved using each of the three general frameworks: FD, SD and DG. In the case of SD and DG, the basis polynomial order was varied, as well as the number of elements. In addition to qualitative comparisons, plots of root-mean-square error (RMSE) versus CPU time and number of degrees of freedom were compiled. Finally, we measured the smallest number of degrees of freedom required for each method (for a particular degree) to achieve a certain order of magnitude of RMSE.

3.1 1D Constant Speed Advection

Constant speed advection is governed by the wave equation: $\frac{\partial u}{\partial t} - c \frac{\partial u}{\partial x} = 0$.

Fig. 3. RMSE in wave equation sine wave solution against CPU time (left) and total number of degrees of freedom (right) for 2nd, 4th and 6th order FD, 6th order DG and 6th order SD

In this case we consider the advection of two initial conditions (one smooth (sine wave) and one nonsmooth (square wave)) through the domain, with periodic boundary conditions. The solutions by the three methods after the sine wave has passed through the domain twenty times (for $c = 1$) are indistinguishable and are therefore not shown. Fig. 3 shows RMSE versus CPU time and the total number of degrees of freedom, for DG and SD taken to be the total number of (solution) nodes. Table 1 shows how many degrees of freedom (nodes) are needed to attain a particular order of magnitude of accuracy. In all cases we compare 6th order DG-LF and SD with central flux against 2nd, 4th and 6th order FD. While higher order will yield better results, we have restricted this presentation to orders typically used in NWP.

Table 1. Degrees of freedom required to achieve an approximate RMSE for the wave equation sine wave solution using FD, DG and SD (2nd, 4th and 6th order)

Order	2 nd			4 th			6 th		
RMSE	SD	DG	FD	SD	DG	FD	SD	DG	FD
10 ⁻¹	18	24	78	10	10	20	7	7	14
10 ⁻²	27	39	246	10	15	30	7	14	14
10 ⁻³	45	69	768	20	20	50	14	14	21
10 ⁻⁴	81	123	2421	25	30	85	21	21	35
10 ⁻⁵	141	231	~8000	40	50	150	42	28	49

3.2 2D Nonconstant Advection – Smolarkiewicz Deformational Flow

In this problem, a temperature bubble is placed into a field of vortices, that then advect the bubble along circular streamlines, following the advection equation:

$$\frac{\partial T}{\partial t} + \frac{\partial}{\partial x}(uT) + \frac{\partial}{\partial y}(vT) = 0 \text{ with } \begin{matrix} u = A \sin(kx) \sin(ky) \\ v = A \cos(kx) \cos(ky) \end{matrix} \text{ and } \begin{matrix} A = 8 \\ k = \frac{4\pi}{100} \end{matrix}.$$

There is a "breaking time" at $t_b = 263.76$ where the gradients become infinitely large. We will examine solutions at $t = t_b / 5 = 52.752$ when the solution exhibits some roll-up and some very fine structures. This problem is relevant to meteorology because it simulates the effects of closed vortices on warm parcels of air. More details can be found in [9], [12] and [13] which provides the exact solution.

Fig. 6 presents the exact solution as well as 6th order FD, SD and DG solutions. The SD results for the 2D Smolarkiewicz flow do not match what we would expect from our 1D advection stability analysis. That is, the central flux case is unstable even for a Courant number of 0.1, while the Lax-Friedrichs flux exhibits no instability at the times investigated. Further, the SD-LF exhibits better errors than the other methods for this test. This is most likely due to the change in character of the Lax-Friedrichs formulation from upwind in the 1D advection case to something more sophisticated in the 2D quasilinear case. The global RMSE results of the DG and SD

solutions are poor, due to severe overshoots near the corners and sharp features in the solution. [Note that while it is possible to adjust the grid and/or use a filter to improve these results, we wanted to present a straightforward comparison of the three methods in this paper, using similar resolution, in order to elucidate the strengths and weaknesses of the respective methods.] However, a spatial map of the error reveals DG to be the best solution overall when matching CPU time and approximately similar number of degrees of freedom, whereas the FD solution is smeared as expected due to the higher diffusion and dispersion errors.

Fig. 4. Plot of nonsmooth (square wave) advection solution with 6th order FD, DG, and SD-LF (35 degrees of freedom)

Fig. 5. RMSE in wave equation square wave solution against CPU time (left) and total number of degrees of freedom (right) for 2nd, 4th and 6th order FD, 6th order DG and 6th order SD-LF

Fig. 6. Smolarkiewicz deformational flow: a) exact solution at time $t_b/5$, and b)-d) numerical solution obtained using 6th order FD, SD-LF and DG respectively (70x70 degrees of freedom) at time $t_b/5$

4 Conclusion

The tests presented show that no one method outperforms the others in a consistent manner. Additional tests in [9] confirm this conclusion. The tests do elucidate the behavior of the different methods however, on different features of advective flows. These are important to keep in mind, especially when resolving at the limit of acceptable resolution.

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