Title: High-Order, Stable, and Conservative Boundary Schemes for Central and Compact Finite Differences

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Stable and conservative numerical boundary schemes are constructed such that they do not diminish the overall accuracy of the method for interior schemes of orders 4, 6, and 8 using both explicit (central) and compact finite differences [2]. Previous attempts to develop stable numerical boundary schemes for non-linear problems have resulted in schemes which significantly reduced the global accuracy and/or required some form of artificial dissipation. Thus, the schemes developed in Ref. [2] are the first to not require this tradeoff, while also ensuring discrete conservation and allowing for direct boundary condition enforcement. After outlining a general procedure for the construction of conservative boundary schemes of any order, a simple, yet novel, optimization strategy which focuses directly on the compressible Euler equations is applied. The result of this non-linear optimization process is a set of high-order, stable, and conservative numerical boundary schemes which demonstrate excellent stability and convergence properties on an array of linear and non-linear hyperbolic problems [1].

Background and Motivation

High fidelity simulations of flow problems (such as Direct Numerical Simulations) are usually performed more efficiently using high order methods. For example, conservative, high-order numerical methods are, in principle, well suited to the challenge of accurately resolving the broadband physics of turbulence over long periods of time. In practice, however, numerical stability is not easily achieved for high-order methods. In particular, when high order finite differences are used, the computational stencil used in the interior must be altered near the computational boundary for non-periodic domains.

Designing high-order numerical boundary schemes such that they are stable for non-linear problems is a very difficult task. The most prevalent solution to this problem is to simply reduce the order of the boundary stencils by roughly half. The problem with this approach is that the overall order accuracy will be limited to 1 more than the boundary stencils. Thus, pursuing a high-order interior scheme while maintaining a significantly reduced order at the boundary is not particularly efficient.

The search for stable, high-order boundary schemes has a long history and is still an active field. The constraints imposed by high fidelity, DNS-type calculations, have motivated the search for an alternate approach targeting the construction of stable, high-order, and conservative numerical boundary schemes which do not require modifications of the grid near the boundaries, artificial dissipation, or weak enforcement of the boundary conditions. Conservative schemes of overall accuracy of orders 4, 6, and 8 (where the order of the numerical boundary schemes is one less) are developed for both explicit and compact finite differences. This is achieved through a simple, yet novel, optimization strategy where we optimize directly on the non-linear Euler equations rather than attempting to utilize a linear stability theory. The procedure relies on the introduction of enough free parameters in the boundary stencils such that the problem admits solutions.

Numerics

In the interior of the domain, standard central and compact finite differences are used to approximate the spatial derivatives. For these schemes, a stencil of order $2(p+s)$ and centered at point i on a grid with constant spacing h, has the form,

$$\sum_{k=-s}^{k=s} \delta_k f_{i+k}^{(\nu)} = \frac{1}{h^\nu} \sum_{j=-p}^{j=p} \gamma_j f_{i+j} + O\left(h^{2(p+s)}\right), \tag{0.1}$$

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where $\delta_0 = 1$, and f are the known function values used to approximate the derivative, $f^{(\nu)}$. However, the interior schemes cannot be used at the first (or last) p points since they would extend beyond the boundaries of the computational domain. Instead, a set of r modified boundary stencils (where $r \geq p$) of order q are used to close the discrete system.

A stencil of order q and width t approximating the first derivative operator at point i, near the left boundary (i.e. $i < r$), can be written as:

$$\sum_{k=-s_1}^{k=s} \beta_{ik} f'_{i+k} = \frac{1}{h} \sum_{j=0}^{j=t-1} \alpha_{ij} f_j + O(h^q) , \qquad (0.2)$$

where $s_1 = \min(i, s)$, and $\beta_{i0} = 1$.

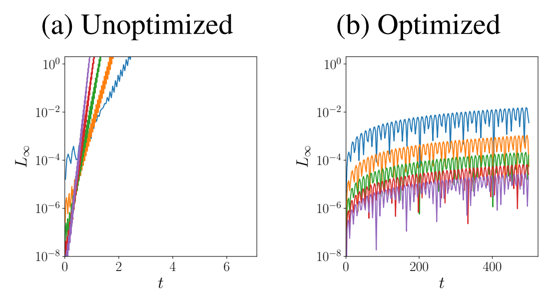
In general, r and t can take a wide range of values and can be chosen such that the resulting boundary schemes have an appropriate number of free parameters.

Main Results and Conclusions

The values of the free parameters have a strong impact on the stability of the system. A novel optimization procedure was developed to find values for these free parameters. The optimization procedure is based directly on evaluating the performance of the boundary schemes in solving the non-linear Euler equations rather than a simplified model problem. This process resulted in a number of schemes which were then subjected to a variety of stability tests, both linear and non-linear. As an example, an unoptimized scheme applied to a challenging hyperbolic test problem is shown in Fig. 1 (a). This scheme results in a very unstable discretization as evidenced by the rapidly diverging error. In contrast, Fig. 1 (b) shows the performance of one of the optimized schemes, demonstrating the success of the optimization procedure.

The schemes presented in [2] are able to achieve high-order and satisfy conservation without introducing artificial dissipation or filtering. The stability and accuracy of the new conservative schemes was verified in a number of ways and compared to three popular schemes existent in the literature. None of the comparison schemes passed all of the stability tests.

To the best of our knowledge, the 6^{th} and 8^{th} order schemes developed in [2] mark the first successful application of conservative finite-differences of such high order to non-linear hyperbolic initial boundary value problems without requiring artificial dissipation or filtering, while allowing for direct boundary condition enforcement.



Error vs Time for applying (a) unoptimized 6^{th} order scheme and (b) optimized 8^{th} order scheme, to a neutrally stable hyperbolic test problem at several grid resolutions (indicated by color). In (a), the instability of the unoptimizied discretization is seen in the rapidly diverging errors. In (b), the error remains bounded for long times, indicating stability

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References

[1] P.T. Brady & D. Livescu. Coefficient dataseets for high-order, stable, and conservative boundary schemes for central and compact finite differences. *Data in Brief*, 2019.

[2] P.T. Brady & D. Livescu. High-order, stable, and conservative boundary schemes for central and compact finite differences. *Computers and Fluids*, 2019.