Approximating derivatives on nonuniform grids using polynomial fitting for receptivity computations of hypersonic flows

By T. J. Flint AND P. Moin

The accurate approximation of derivatives on highly nonuniform grids for the solution of hyperbolic equations is important for receptivity computations in hypersonic flows. The application of high-order central differences, along with a grid transformation, results in an unstable scheme for the linear advection equation. If instead the derivatives are approximated from a polynomial fit to the data at the grid points, the scheme is stable. This research brief presents the stability and modified wavenumbers of these two schemes.

1. Introduction

Stability calculations in hypersonic flows have a number of characteristics that make them difficult to solve numerically. This brief discusses a particular method for finite-difference approximation of derivatives that is well suited for this problem.

In the design of hypersonic transatmospheric vehicles, the method used to estimate the location of transition can change the weight of the vehicle by as much as 50% (Anderson 2006). Although relatively old now, this example highlights the difficulty and importance of transition prediction in hypersonic flows, a regime in which models still rely on calibration by flight data of similar vehicles.

The dependence on the freestream disturbance environment has complicated both experimental and theoretical analyses of transition in high-speed flows (Reshotko 1976). Calculations to study receptivity and transition in hypersonic flows must overcome a number of challenges: High accuracy is often desirable so that traveling waves and instabilities can be resolved efficiently, shocks must be treated, the length over which transition occurs is long compared with length scales near the leading edge of the geometry, the equations can be hyperbolic in some parts of the domain and subject to minimal physical dissipation, and time-accurate solutions are required. A suitable choice that offers high accuracy is the use of a structured grid. The structured grid must be nonuniform so as to conform to the geometry and to efficiently resolve boundary layers and shocks. Due to geometric disparities in length scales, the structured nature of the grid forces the grid in some regions of the domain to be far smaller than the physical length scales of interest, which makes for an unnecessarily stiff system. Numerically stable discretization of hyperbolic systems often requires special treatment in order to be stable for complex cases. A number of receptivity and transition calculations of transition on hypersonic cones have chosen to use high-order schemes on a structured grid with some form of upwinding for stabilization and in combination with domain decomposition into a number of zones (up to 35 in the references listed), which are one-way coupled to overcome the numerical stiffness of the small grid size near the nose of the cone (Zhong & Ma 2006; Kara *et al.* 2007; Wan *et al.* 2020; Schuabb *et al.* 2025; Varma & Zhong 2025).

The discretization of the linear advection equation on a stretched grid in the uniform, transformed, computational space with a central-difference scheme produces an unstable solution on a grid that expands in the advection direction. Zhong (1998) observed this instability when using a high-order upwind-biased scheme on a stretched grid and found that it was stabilized through the use of a nonuniform discretization instead of a grid transformation. This brief discusses the discretization of the linear advection equation using a typical (i.e., no explicit upwinding added) nonuniform finite-difference scheme, as opposed to a grid transformation. This discretization is stable in the presence of grid stretching, collapses to the typical central scheme on uniform grids, and lends itself to implicit time advancement. Compared with the current commonly used methods, the proposed method has the potential to offer a solution that is less dissipative, can handle more severe grid stretching, and does not require a domain decomposition in order to overcome numerical stiffness.

2. Finite-difference methods on nonuniform grids

2.1. *Grid transformation*

Using a grid transformation to map the physical space, x, to a computational space, ξ, where the grid is uniform and orthogonal, results in the discrete first derivative operator in one dimension,

$$D_{gt} = \mathrm{diag}\left(\frac{d\xi}{dx}\right) D_{fd}, \tag{2.1}$$

where D_{fd} is any difference operator derived for a uniform grid and $d\xi/dx$ is the grid metric of the transform.

2.2. *Polynomial fitting*

Fitting a polynomial to a number of grid points, and then evaluating the derivative of this interpolating polynomial, is another way of constructing finite-difference operators on nonuniform grids (e.g., Ferziger *et al.* 2019). The order of accuracy for the approximation of the first derivative is equal to the order of the polynomial used to approximate the function. For second derivatives, the order of accuracy is equal to the degree of the interpolating polynomial minus one, with an extra order gained on uniform grids when even-order polynomials are used. Here, we consider fitting curves to equal points on either side of the target point. Performing the fit on the basis of the distance from the central point, as opposed to its location, reduces conditioning problems arising from the polynomial fit.

3. Equation of interest

The problem used to test the schemes is the one-dimensional constant-coefficient linear advection equation,

$$\frac{d\phi}{dt} = -\frac{d\phi}{dx}, \tag{3.1}$$

with the boundary condition

$$\phi(x = 0) = 0. \tag{3.2}$$

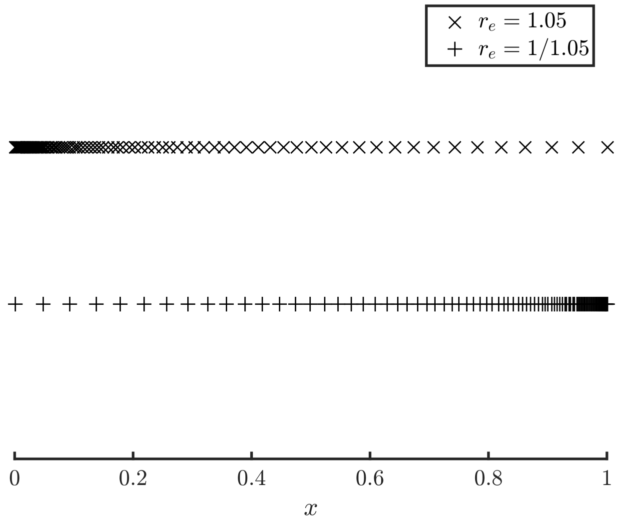

FIGURE 1. Grid points for two grids with different stretching factors, r_e, and with $N = 100$ grid points.

4. Grid choice

Equation (3.1) is solved on a compound-interest grid, where the grid expands or contracts with a constant factor, r_e,

$$x_{j+1} - x_j = r_e(x_j - x_{j-1}). \tag{4.1}$$

Figure 1 shows the grid points for $N = 100$ grid points with $r_e = 1.05$ and $r_e = 1/1.05$.

5. Comparison of scheme stability

5.1. *Scheme details*

Here we compare the stability of fourth-order finite-difference schemes using the two methods, grid transformation and polynomial fitting. The tests used a discretization with $N = 100$ grid points.

5.1.1. *Grid transformation*

The grid transformation method uses a fourth-order central-difference scheme for the first derivative in the computational coordinate system with third-order one-sided and mixed-sided schemes at the boundary points and the points immediately interior from the boundary, respectively. The grid metrics are computed discretely using the above-mentioned scheme.

5.1.2. *Polynomial fitting*

The polynomial fitting method tested here approximates the first derivative using a fourth-order polynomial fit to five points with indices $j-2, j-1, j, j+1$, and $j+2$, where j is the index of the location at which the derivative is to be approximated. Near the boundaries, a third-order polynomial fit at the second point from the boundary is used to approximate the derivatives at the boundary points and those immediately interior.

Method	$max(\lambda_r)$
Grid expanding in the direction of flow, $r_e = 1.05$	
Grid transformation	128 (unstable)
Polynomial fit	−7.03
Grid contracting in the direction of flow, $r_e = 1/1.05$	
Grid transformation	−7.09
Polynomial fit	−1.82
Uniform grid, $r_e = 1$	
Grid transformation	−0.000358
Polynomial fit	−0.000358

TABLE 1. Largest real part of the eigenvalue, $max(\lambda_r)$, for the two fourth-order schemes on different grids.

5.2. *Eigenvalues with the largest real part*

We compare the stability of the schemes by computing the eigenvalues of their respective discrete representations on the right-hand side of Eq. (3.1). Table 1 presents the eigenvalues with the largest real part for a number of tests; a value of $\lambda_r > 0$ indicates an exponentially unstable semidiscrete solution.

The results show that using a grid transformation on a grid that expands in the direction of the advection velocity results in an unstable semidiscrete system, while using the polynomial fitting discretization results in a stable solution on all grids tested.

6. Modified wavenumber analysis

Assuming a sinusoidal ansatz, one can compute a modified wavenumber resulting from the discrete approximation of the derivative,

$$\frac{d\phi}{dx} = \mathrm{i}ke^{\mathrm{i}kx}, \tag{6.1}$$

$$\approx \Big[a_{j,-2}e^{\mathrm{i}k(x_{j-2}-x_j)} + a_{j,-1}e^{\mathrm{i}k(x_{j-1}-x_j)} \tag{6.2}$$

$$+ a_{j,0} + a_{j,+1}e^{\mathrm{i}k(x_{j+1}-x_i)} + a_{j,+2}e^{\mathrm{i}k(x_{j+2}-x_j)}\Big]e^{\mathrm{i}kx_j} \tag{6.3}$$

$$= \mathrm{i}\hat{k}_j e^{\mathrm{i}kx_j}, \tag{6.4}$$

where $\hat{k}$ is the modified wavenumber and $a_{j,k}$ is the finite-difference coefficient for the $(j + k)$th point of the approximation to the derivative at the jth grid point. Because

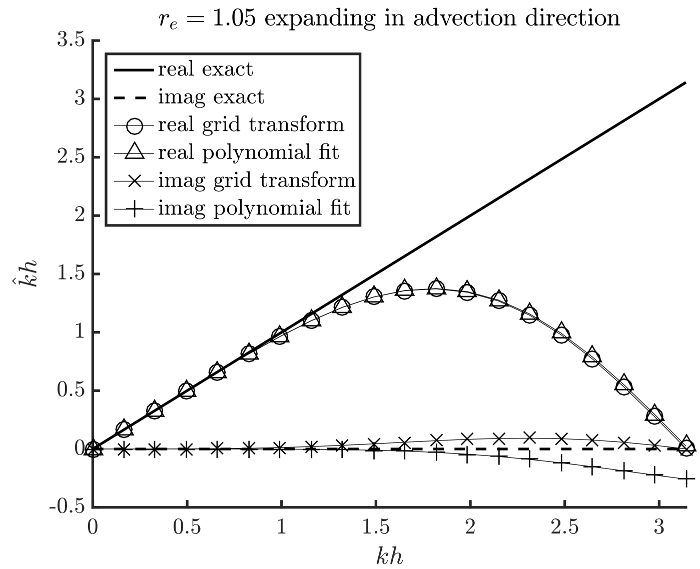

FIGURE 2. Modified wavenumber for the two discretization schemes on a grid with $r_e = 1.05$, expanding in the advection direction.

the grid is nonuniform, the modified wavenumber is in general a function of the location at which the derivative is being approximated, j. However, one can show that, for the compound-interest grid used here, when the modified wavenumber is normalized by the average grid spacing of the five-point stencil, h_j, it is independent of the location, j, and simply a function of the expansion ratio, r_e.

Figures 2, 3, and 4 show the real and imaginary parts of the modified wavenumber for the expanding, uniform, and contracting grids, respectively. On a uniform grid, both schemes collapse to the fourth-order central-difference modified wavenumber, with zero imaginary part. When the grid is stretched, both methods have complex modified wavenumbers; a similar result has been observed for compact schemes on stretched grids (Gamet *et al.* 1999) and does not necessarily imply numerical instability, as demonstrated in Section 5.2. The imaginary part of the modified wavenumber departs from zero earlier for the grid transformation–based scheme. The imaginary part of the modified wavenumber reaches a higher value at high wavenumbers for the polynomial-based scheme, while the grid transformation–based scheme returns to zero at the grid scale.

7. Conclusions

The widely used discretization of the first derivative on a nonuniform grid using a grid transformation and a fourth-order central-difference scheme is unstable when applied to the linear advection equation on a grid that expands in the direction of the flow. An alternative discretization that directly includes the effect of the nonuniform grid in the coefficients through polynomial fitting is stable for the linear advection equation on stretched grids. Both schemes have complex modified wavenumbers on stretched grids. The polynomial fitting method departs from the exact wavenumber later than the grid transformation, although it eventually deviates more at high wavenumbers.

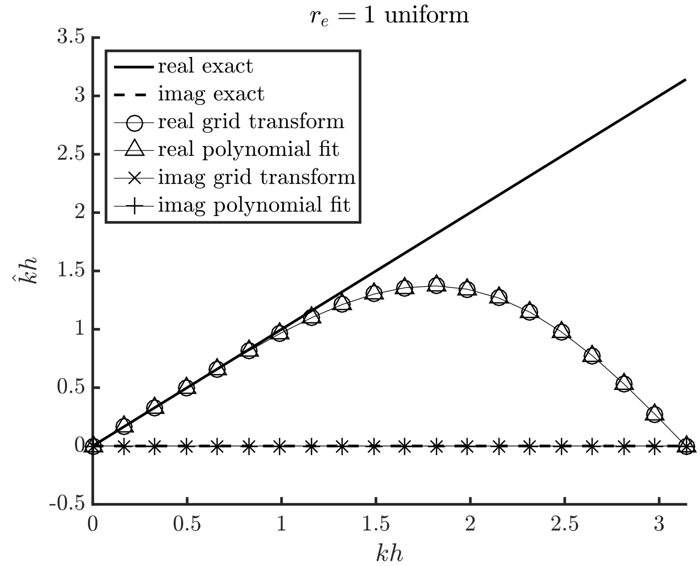

FIGURE 3. Modified wavenumber for the two discretization schemes on a grid with $r_e = 1$, uniform.

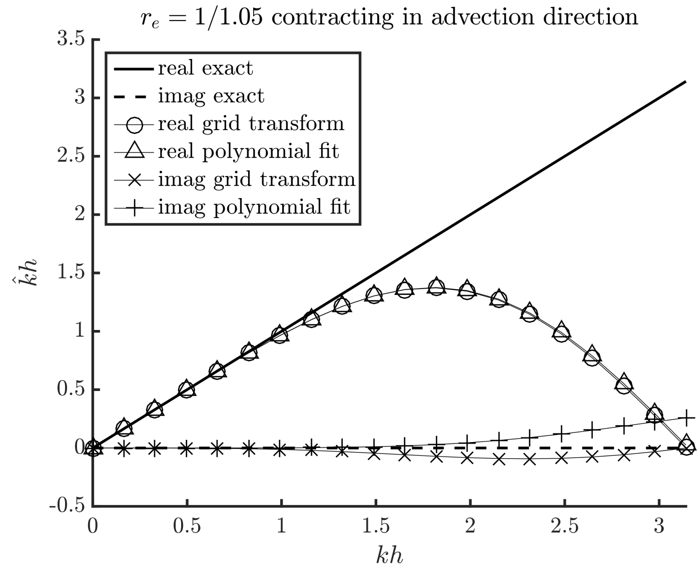

FIGURE 4. Modified wavenumber for the two discretization schemes on a grid with $r_e = 1/1.05$, contracting in the advection direction.

Acknowledgments

This investigation was funded by a Franklin P. and Caroline M. Johnson Fellowship in the School of Engineering at Stanford University.

REFERENCES

ANDERSON, J. D. JR. 2006 *Hypersonic and High-Temperature Gas Dynamics.* American Institute of Aeronautics and Astronautics. 2nd ed.

FERZIGER, J. H., PERIĆ, M. & STREET, R. L. 2019 *Computational Methods for Fluid Dynamics* 4th ed. Springer.

GAMET, L., DUCROS, F., NICOUD, F. & POINSOT, T. 1999 Compact finite difference schemes on non-uniform meshes. Application to direct numerical simulations of compressible flows. *Int. J. Numer. Methods Fluids* **29**, 159–191.

KARA, K., BALAKUMAR, P. & KANDIL, O. A. 2007 Effects of nose bluntness on stability of hypersonic boundary layers over a blunt cone. *AIAA Paper 2007-4492.*

RESHOTKO, E. 1976 Boundary-layer stability and transition. *Annu. Rev. Fluid Mech.* **8**, 311–349.

SCHUABB, M., DUAN, L., CASPER, K. M., WAGNILD, R. M., CHOUDHARI, M. M. & PAREDES, P. 2025 Hypersonic boundary-layer transition over a circular cone in a Mach 8 digital wind tunnel. *J. Fluid Mech.* **1017**, A33.

VARMA, A. R. & ZHONG, X. 2025 Hypersonic boundary-layer receptivity to free-stream acoustic waves with thermochemical non-equilibrium effects. *J. Fluid Mech.* **1013**, A16.

WAN, B., SU, C. & CHEN, J. 2020 Receptivity of a hypersonic blunt cone: role of disturbances in entropy layer. *AIAA J.* **58**, 4047–4054.

ZHONG, X. 1998 High-order finite-difference schemes for numerical simulation of hypersonic boundary-layer transition. *J. Comput. Phys.* **144**, 662–709.

ZHONG, X. & MA, Y. 2006 Boundary-layer receptivity of Mach 7.99 flow over a blunt cone to free-stream acoustic waves. *J. Fluid Mech.* **556**, 55–103.