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Investigating the use of Walsh functions for computing flows with unsteady shocks

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Abstract

A new numerical treatment for flows with shocks proposed by Gnoffo [3, 4] is independently implemented and its suitability assessed for the simulation of unsteady flows with shocks. The method combines strengths from both shock-tracking and shock-fitting, and is applied to a static, structured grid. This paper details the specifics of implementing the method for the advection equation, with the larger goal of applying it to the simulation of expansion tubes that produce hypersonic test flows. The new method, based on Walsh functions, is compared to a conventional finite-volume method of low order to provide insight on whether the new method is worth pursuing for multi-dimensional flows.

Introduction

There are two commonly used techniques to treat shock waves in the numerical simulation of compressible flows: shock-capturing and shock-fitting. The former works by allowing the discretisation technique within a given compressible flow code to handle the development of the discontinuity and the subsequent transfer of information from flow variables either side. As no extra schemes or data structures are required in terms of a regular finite volume method, the shock-capturing approach is easy to implement. This points to the method's limitations: as a result of the numerical methods handling the change of flow variables across the shock, data points can occur between the pre- and post-shock states which are a numerical artefact and do not reflect the shock shape [8]. Low-order methods are diffusive, so when handling shocks they cannot capture the sudden change in properties and the result is smearing of shock information across multiple cells. High-order methods are less diffusive and can better capture the near discontinuous change, but do so at the cost of introducing ripples of overshoots and undershoots in the flow properties, known as Gibb's phenomenon. Limiters, a significant achievement in CFD history [6], work to prevent these overshoots and undershoots by limiting the gradient or preventing new extremities. A drawback of limiters is that locally, downwind of the shock they reduce the scheme to first order. Another drawback is that extrema in the flow are locally deformed by the limiter [6].

Shock-fitting treats shocks as a boundary with no transfer of information through interpolation for fluxes or gradient calculation schemes. Instead, exact Rankine-Hugoniot relations are applied across the shock to determine the flow variables on either side. The difficulty with shock-fitting is in locating the shock with high accuracy and tracking its movement through the domain (including interactions with other shocks or edges), as the grid needs to align well with the shock. A floating shock-fitting method was developed by Moretti [7] whereby the shock is allowed to move through the points of a fixed grid and is treated as an internal boundary [2]. This helped avoid the requirement of moving the grid, but it was found to not be robust and require 'a heavy, patient and handcraft' effort by the researchers [8]. Further work into floating shock-fitting for unstructured grids [9, 10, 1] has shown promising results, but as best practices maintain that the cell faces should be perpendicular or parallel to shocks [4], methods for shock-fitting on structured grids should still be investigated.

A floating shock-fitting and shock-tracking method recently proposed by Gnoffo [4] has the potential to improve current methods for a structured grid. The present work is an independent implementation of that method and a comparison to a one-dimensional code with conventional finite-volume schemes. These conventional schemes are representative of the schemes we presently have available in the compressible flow solver, Eilmer [5]. As such the comparison between the new hybrid method and the conventional schemes will serve to inform whether the new method is worth pursuing in our production code. The new method applies discontinuous basis functions to interpolate through a set of discrete data at regular spacing, providing a correction to the gradients and enabling detection and tracking of shocks. The larger goal of this work is to apply the shock-tracking method to the simulation of expansion tubes for hypersonic test flow production. A critical feature of those simulations is the ability to track and adequately resolve a travelling shock over a large physical domain on the order of tens of metres.

Numerical Method

Polynomial curve fit with Fast Walsh Transform

Walsh functions are a closed set of orthogonal functions [12] that exhibit closure under multiplication, and they have been shown to be capable of detecting features in flow such as discontinuities [4]. Gnoffo's past work on solving flow problems with Walsh functions [3, 4] provides explanations and derivations of the following equations (and the reader is referred to that work for more detail).

A set of 2^p discrete data points f_i and monomials x_i^m can be represented by a truncated series of Walsh functions (g_n) with coefficients A_n and $B_{n,m}$ respectively.

$$f_i = \sum_{n=1}^{2^p} A_n g_n(x_i) \quad \text{where } A_n = \sum_{i=1}^{2^p} g_n(x_i) f_i \Delta x \qquad (1)$$

$$x_i^m = \sum_{n=1}^{2^p} B_{n,m} g_n(x_i) \quad \text{where } B_{n,m} = \sum_{i=1}^{2^p} g_n(x_i) x_i^m \Delta x \qquad (2)$$

The coefficients can be calculated as per equations (1, 2) or by using a fast Walsh transform (FWT) as explained in [4]. Using Gnoffo's shock detection method [4] to find the shock location x^* and height h, a polynomial fit accounting for the shock is given by

$$\tilde{f}(x) = \sum_{k=0}^{m} a_k x^k + hH(x, x^*) \qquad (3)$$

where $H(x,x^*)$ is equal to 0 for $x \le x^*$ and equal to 1 for $x > x^*$. The novel idea in using that FWT fit is that the fit works in smooth regions of the flow to provide interpolation of flow values, and it can be used to detect discontinuities in the flow.

Application to Problems

Gnoffo details a general formulation for solving differential equations with the FWT fit [4]; the formulation for the advection equation is shown here. The model equation for linear advection is

$$\frac{\partial q}{\partial t} + \frac{\partial f}{\partial x} = 0 \tag{4}$$

with $f = cq$, q a scalar, a domain of $0 \leq x \leq 1$ and a periodic boundary condition whereby $q(0,t) = q(1,t)$. The advection wave speed is constant at $c = 1$, thus simplifying the relationship between flux and flow variable to

$$\frac{\partial f}{\partial q} = 1 \tag{5}$$

A semi-discrete numerical form is

$$\frac{dq}{dt} = -\frac{\partial f}{\partial x} = -\frac{1}{\Delta x}\left(f^*_{i+1/2} - f^*_{i-1/2}\right) \tag{6}$$

When there are no shocks present in the stencil, a fourth-order accurate scheme for the numerical flux is incorporated such that

$$\frac{dq}{dt} = -\frac{1}{24\Delta x}(27(f_{i+1/2} - f_{i-1/2}) - (f_{i+3/2} - f_{i-3/2})) \tag{7}$$

The fluxes at the cell interfaces are now calculated from the values at the cell centres using interpolation that incorporates the FWT polynomial fit. A FWT fit is applied over a set of discrete q_i cell centre data points, and from that the FWT fit data points at the cell centre $\tilde{q}_i$ and the cell interfaces $\tilde{q}_{i+1/2}$ are obtained. It has been shown [4] that the FWT polynomial fit breaks down when there are multiple extrema in the flow, and the method can only detect two shocks within a fit. Thus multiple overlapping FWT fits are applied over the domain, with the final cell interface variable and thus cell interface flux selected from the appropriate FWT fit after. For each FWT fit, the following process provides a correction to the cell interface value. The correction at the cell centre is

$$\delta q'_i = \delta q_i = q_i - \tilde{q}(x_i) \tag{8}$$

which can then be interpolated to obtain the correction at the cell interface (no boundary treatment is required as the end values will not be selected later)

$$\delta q'^{+}_{i+1/2} = L(\delta q'_{i+1}, \delta q'_i, \delta q'_{i-1}, \delta q'_{i-2}) \tag{9}$$

$$\delta q'^{-}_{i+1/2} = L(\delta q'_i, \delta q'_{i+1}, \delta q'_{i+2}, \delta q'_{i+3}) \tag{10}$$

An interpolation stencil for evenly spaced cells is

$$L(a,b,c,d) = (5a + 15b - 5c + d)/16 \tag{11}$$

The corrections to the fluxes at the interfaces are now determined — for advection to the right only the upwind flux is required.

$$\delta f^{+}_{i+1/2} = \delta q'^{+}_{i+1/2} \tag{12}$$

$$\delta f^{-}_{i+1/2} = 0 \tag{13}$$

And finally the corrected cell interface flux value is

$$f_{i+1/2} = \tilde{f}(\tilde{q}(x_{i+1/2})) + \delta f^{+}_{i+1/2} + \delta f^{-}_{i+1/2} \tag{14}$$

Overlapping FWT fits are applied over the domain to reduce the introduction of non-physical features caused by interpolation through discontinuities where successive FWT fits meet. Figure 1 shows a stencil for the fluxes modified from [4]. For a domain with n elements there will be n 'elemental' FWT fits as shown in the black (top), and n 'blended' FWT fits as shown in red (bottom) and a second blended fit (not shown) at the periodic boundary. The correction process described above is applied along the length of each FWT fit, and after calculating the interpolation from the cell centres to the cell faces sections of each FWT fit are chosen for the final value. Testing and comparison to the exact flux ($f = q$) demonstrated that it was not possible to achieve accurate fluxes if selecting flow data from each FWT prior to interpolation. Only information (cell centres and interfaces) between $N_a/4$ and $3N_a/4-1$ (0 index) from the elemental FWT are used, and within $N_a/4$ of an elemental boundary from the blended FWT fit - the rectangular blocks show the regions where the flow properties are selected from the respective fits. Note the distinction here - the FWT fit over the interface between two elements is referred to as the 'blended' FWT fit, but there is no combining of the values between the elemental and blended FWT fits.

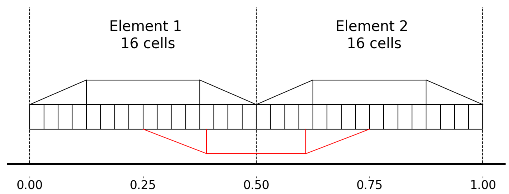

Figure 1: Stencil showing locations of elemental FWT fits (top) and blended FWT fits (bottom). The FWT fits are applied using cell centre information from every point within their element, however at a later stage only the regions within the rectangular regions are selected from each FWT fit. Modified from Gnoffo [4]

Using a time-integration method such as Runge-Kutta (RK) to advance the system, the process for each iteration beginning with the cell centred flow variables is:

- apply a FWT polynomial fit across the cell centred flow variables (q_i) in each element (including the blended elements), obtaining $\tilde{q}_i$ and $\tilde{q}_{i+1/2}$;
- for each step in the RK updater, using the new pseudo variables (i.e. q passed to the RK):
  - calculate corrections between the FWT fit cell centre flow variables, along the length of each fit;
  - interpolate along each FWT fit to obtain the corrections at the cell interfaces - disregard the end points missed by the interpolation stencil;
  - using the element stencil shown in Figure 1 and described previously, select the appropriate values from the appropriate sections of the cell interface corrections from the element and blended FWT fits;
  - calculate corrections to the cell interface invisid flux values from the cell interface corrections;
  - update inviscid fluxes using corrections from the FWT interpolation information;
  - calculate flux difference terms; and,
  - update RK pseudo variables.
- obtain new cell centred flow variables.

Finite Volume Method for Comparison

To compare Gnoffo's scheme using FWT fits to more conventional method, we chose some finite-volume (FV) schemes of 2nd- and 3rd-order spatial accuracy. These FV schemes are representative of the current technology available in the flow solver, Eilmer. So the comparison will provide some insights on the benefits or otherwise of developing Gnoffo's method in multidimensions for our production code. The selected FV schemes are Fromm's scheme (2nd order) and a 3rd-order scheme from Hirsch [6]. The van Albada limiter was used in the FV schemes when doing the advection problem with a C0 discontinuity.

For all spatial schemes, a fourth-order Runge-Kutta temporal scheme was used. Keeping a consistent temporal scheme allows the comparison to focus on the spatial accuracy offered by the various methods.

Results and Discussion

To enable verification of this implementation with Gnoffo's results, three profiles as suggested by Gnoffo were advected 20 times across a domain with periodic boundary conditions. The three profiles present increasing difficulty to the numerical methods in terms of their discontinuities: (a) a Guassian profile (continuous); (b) a triangular profile (C1 discontinuity); and (c) a cosine profile with Heaviside function jump (C0 discontiuity). These test profiles for advection are shown in Figure 2. To determine spatial accuracy, solutions were computed on various grids of increased refinement.

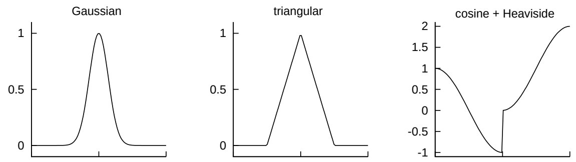

Figure 2: Test profiles for advection equation.

Cell sizes were kept constant between the different schemes, and reduced by powers of 2 for each refinement. Figures 3–7 show the 1-norm error for the Gaussian, triangular, and cosine with jumps profiles respectively.

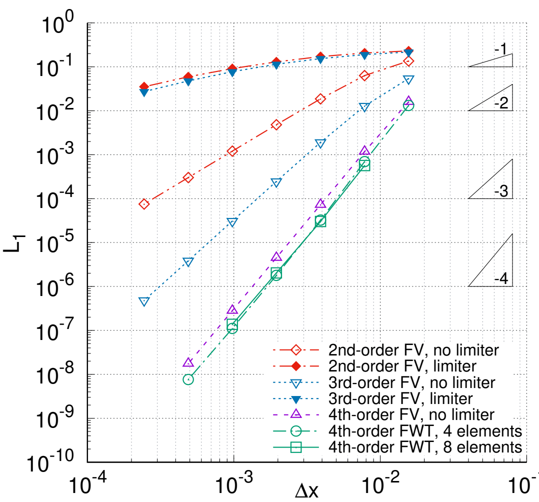

Figure 3: L_1 error comparison for advection of a Gaussian profile, 20 times across a domain with a cyclic boundary condition.

For the Gaussian profile, the second-, third-order FV schemes and the fourth-order FWT method all display 2nd-, 3rd- and 4th-order error convergence behaviour, as expected. The application of limiters to the second- and third-order schemes reduces the accuracy of the solution around the extrema region of the Gaussian profile, resulting in significantly reduced accuracy (to approximately 1st order). The fourth-order scheme with FWT interpolation corrections performs better than the fourth-order scheme without. As noted by Gnoffo [4], a scheme with four

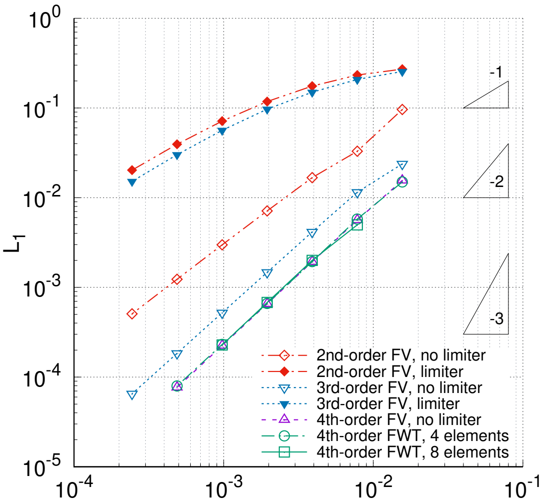

Figure 4: L_1 error comparison for advection of a triangular profile, 20 times across a domain with a cyclic boundary condition.

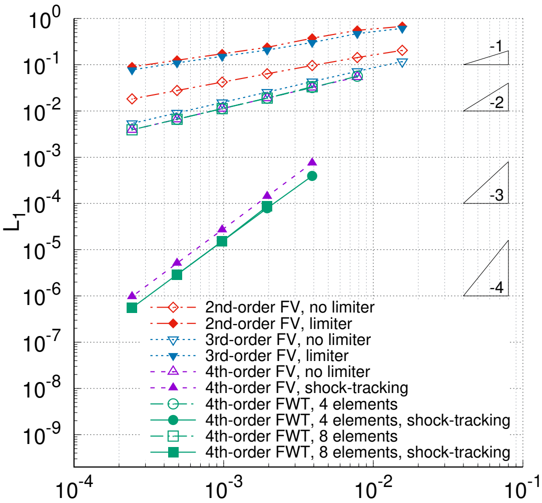

Figure 5: L_1 error comparison for advection of a cosine profile with two discontinuities of height 1, 20 times across a domain with a cyclic boundary condition.

elements and 2^p cells per element has similar accuracy to a scheme with eight elements and 2^{p-1} cells per element.

The triangular profile shows similar results, with the exception that the fourth-order scheme with the FWT interpolation shows no improvement over the same scheme without the FWT fit. This may be solved by the detection of C1 discontinuities, which Gnoffo has now implemented. In the advection of the cosine profile (with jumps) there is little difference between the order of convergence of the 1-norm, but the higher order methods are still more accurate. The fourth-order method with shock-tracking offers significant advantage over the other methods, and improves on the fourth-order scheme without FWT corrections. It can be seen in Figure 6 that both of these methods are almost indistinguishable from the analytical solution after a single cycle of the domain. The order of convergence for the 1-norm for the fourth-order shock-tracking is -2.39.

Conclusions

Gnoffo's method of feature detection and interpolating with FWT has demonstrated increased levels of accuracy for the ad-

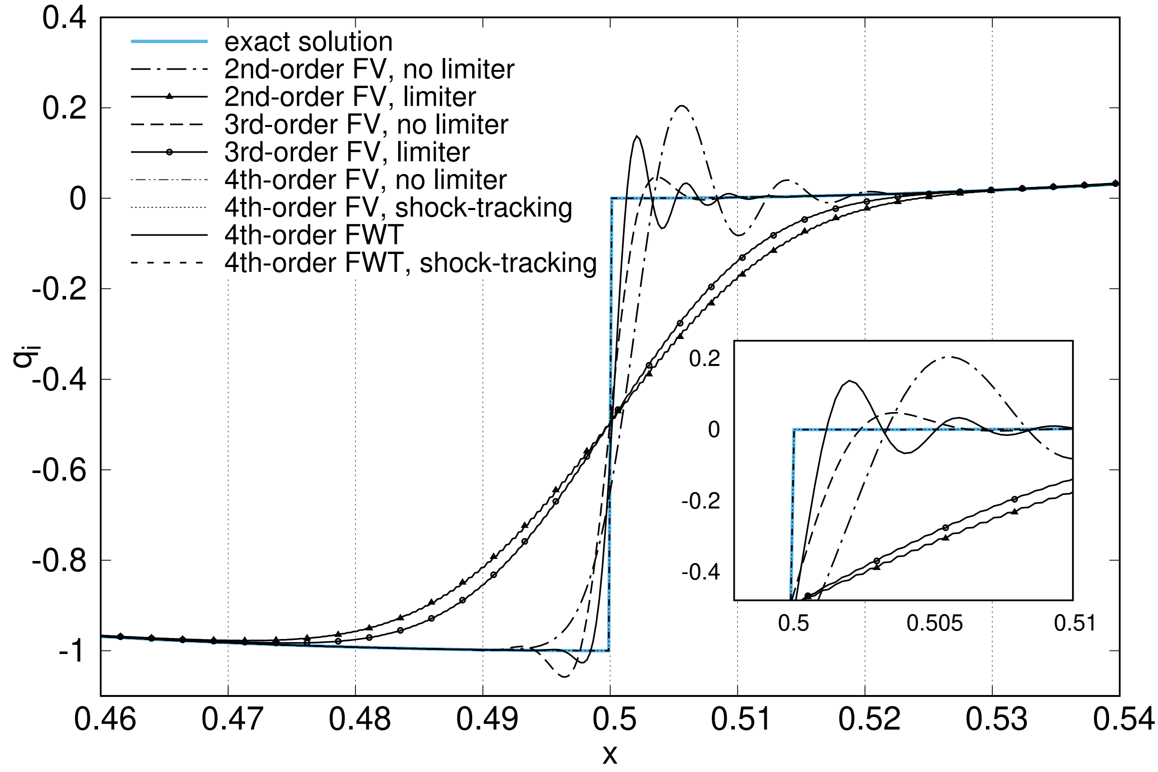

Figure 6: Comparison of different methods and schemes at the discontinuity in the cosine with jumps profile, after being advected once across the periodic domain. Insert shows the top of the shock in more detail — note that lines for '4th-order FV' and '4th-order FWT' overlap each other. The lines for '4th-order FV, shock-tracking' and '4th-order FWT, shock-tracking' do as well.

vection equation with shocks. The implementation of Gnoffo's method has been verified through comparisons of 1-norm error data. The short term goal is complete testing of the new method as a proof-of-concept in simple one-dimensional problems including Burgers' equation and the Euler equations. If shown viable, the long term goal is use the FWT fit for interpolation and shock-tracking in a production multi-dimensional finite volume code.

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