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Combining Galerkin matrix perturbation with Taylor weak statement algorithms

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Abstract

For a large class of computational fluid dynamics (CFD) problems, the discrete approximate solution error is viewed as truncation of a Taylor series expansion. In this paper, a recently developed weak statement Galerkin Matrix Perturbation (GMP) method, is theoretically compared and combined with the well known Taylor Weak Statement (TWS) algorithm on a term by term basis yielding simple tridiagonal forms that reduce, or annihilate in special cases, the Taylor series truncation error. Verification hyperbolic solution is documented for a linear smooth and non-smooth incompressible wave cluster propagation using a combination algorithm of GMP and TWS. © 2000 Elsevier Science S.A. All rights reserved.

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1. Introduction

Approximate CFD algorithms to the non-diffusive transient (Euler) problem class are characterized by a phase lag dispersion error that can highly distort the approximation solution. The theoretical remedy is to increase the mesh density or algorithm order-of-accuracy. Conversely, the ''practical'' remedy is to add an elliptic perturbation with a (linear or non-linear) numerical viscosity coefficient. A variation involves flux correction operators, to remove induced excessive dissipation via an antidiffusive contribution. The goal is to induce a damping mechanism for control of non- monotonicity, but solutions tend to suffer from excess diffusion even on a dense mesh. Detailed comparisons of this phenomenon for the 1-D and 2-D linear convection verification problems are available, cf. [1–5].

For the state variable q, the kinetic flux vector $\mathbf{f} = \mathbf{u}q$, with convection velocity u, the dissipative flux vector $\mathbf{f}^v = \epsilon \partial q/\partial \mathbf{x}$, with diffusion coefficient ϵ, and the source term s, the multidimensional form of the general equation is

$$\mathscr{L}(q) = \frac{\partial q}{\partial t} + \frac{\partial(\mathbf{f} - \mathbf{f}^v)}{\partial \mathbf{x}} - s = 0, \text{ on } \Omega \times t \subset \mathscr{R}^d \times \mathscr{R}^+, \ 1 \leqslant d \leqslant 3. \tag{1}$$

The Fourier representation of the analytical solution to the multidimensional non-diffusive (i.e., $\epsilon = 0$) Euler form of the general Eq. (1) is a sum series of $A e^{i\omega_z(\mathbf{x}-\mathbf{u}t)}$ where ω_z is the wave number of zth wave and A's are the expansion coefficients. Hence, the exact solution for any finite Fourier mode is $\exp(i\omega(\mathbf{x} - \mathbf{u}t))$. The phase dispersion error of the numerical solution is related to real part of the convective $\mathbf{u}$ while the dissipation error is related to the imaginary part of $\mathbf{u}$.

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The algorithm amplification factor G determines how the fully discrete solution grows or decays in time, for the temporal and spatial discretization measure δt and δx, the analytical amplification factor is

$$G = \exp(-\mathrm{i}w\mathbf{u}(n\delta t)) = \exp(-\mathrm{i}mC). \tag{2}$$

In 1-D, $G = \exp(-\mathrm{i}mC)$. Using Laurent series expansion on m with a_l coefficients, one may write

$$G = \sum_{l=0}^{\infty} a_l m^l = 1 - \mathrm{i}mC - \frac{(mC)^2}{2!} + \frac{\mathrm{i}(mC)^3}{3!} + \frac{(mC)^4}{4!} - \cdots, \tag{3}$$

where $m = \omega\delta x$ is the virtual non-dimensional wave number with $C = u\delta t/\delta x$ the corresponding Courant number.

The discrete approximation solution amplification factor G^h is algorithm specific and may be computed via a Fourier modal analysis of the discretized CFD recursion relation. The order of accuracy, hence stability, of a numerical algorithm may be determined from its amplification factor G^h by matching coefficients of powers in wavenumber in the Laurent series expansion with the analytical solution G in Eq. (3).

Independent of the domain dimension, for general variation of physical properties and the flux vector, the semi-discrete finite element (FE) weak statement always yields an ODE system of the form

$$\mathcal{W}S^h = [M]\{Q(t)\}' + \{R\} = \{0\}, \tag{4}$$

$$[M] = S_e[M]_e, \tag{5}$$

$$\{R\} = S_e(([U]_e + [D]_e)\{Q(t)\}_e - \{b(t)\}_e), \tag{6}$$

where $\{Q(t)\}$ is the time-dependent discrete approximation nodal coefficient set. $\{Q(t)\}'$ denotes $\mathrm{d}\{Q\}/\mathrm{d}t$, which may be replaced by using a θ-implicit or n-step Runge–Kutta time integration procedure. S_e symbolizes the "assembly operator" carrying local matrix coefficients into the global arrays. $[M] = S([M]_e)$ is the "mass" matrix associated with element level interpolation, the $[U]_e$ matrix carries the element convection information, $[D]_e$ is the diffusion matrix resulting from genuine (not for Euler) or numerical elemental viscosity effects, and $\{b\}$ contains all known data.

2. Galerkin matrix perturbation (GMP) algorithm

Assuming that an arbitrary order of the Taylor series truncation error for the temporal and spatial discretization may be expressed in the form of FE perturbation matrices, the temporal and convection matrices of linear basis rank form become

$$[M] = S_e([M]_e - [\mathrm{APERT}]_e) \tag{7}$$

$$\{R\} = S_e(([U]_e - [\mathrm{APERX}]_e)\{Q(t)\}_e - b(t)), \tag{8}$$

where $[\mathrm{APERT}]_e$ and $[\mathrm{APERX}]_e$ are element level pertubation matrices that may be determined via comparing the Laurent series of the algorithm G^h and matching arbitrary coefficients for order accuracy with the Laurent series of G in Eq. (3), [6]. The forms of the elements of $[\mathrm{APERT}]_e$ and $[\mathrm{APERX}]_e$ are a sum series of $a_r \exp(\mathrm{i}mr), 0 \leqslant r \leqslant \alpha, \beta, \gamma, \delta$, where a's are determinable coefficient and $\alpha, \beta, \gamma, \delta$ estimates the order of accuracy of the algorithm. Details for arbitrary order-accurate algorithms are available in Ref. [6].

The resulting temporal (7) and convective (8) matrices in 1-D are

$$\frac{1}{\Delta x_e}[M]_e = [\mathrm{A200L}] - [\mathrm{APERT}] = \frac{1}{6}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}_{2\times 2} - \frac{1}{6}\begin{bmatrix} \Lambda_1 & \Psi_1 \\ \Gamma_1 & \Upsilon_1 \end{bmatrix}_{2\times 2} = \frac{1}{6}\begin{bmatrix} 2-\Lambda_1 & 1-\Psi_1 \\ 1-\Gamma_1 & 2-\Upsilon_1 \end{bmatrix}_{2\times 2} \tag{9}$$

and

$$\frac{1}{U}[U]_e = [\mathrm{A201L}] - [\mathrm{APERX}] = \frac{1}{2}\begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}_{2\times 2} - \frac{1}{2}\begin{bmatrix} \Lambda_2 & \Psi_2 \\ \Gamma_2 & \Upsilon_2 \end{bmatrix}_{2\times 2} = \frac{1}{2}\begin{bmatrix} -(1+\Lambda_2) & 1-\Psi_2 \\ -(1+\Gamma_2) & 1-\Upsilon_2 \end{bmatrix}_{2\times 2}. \tag{10}$$

In Eqs. (9) and (10), [A200L] and [A201L] remain the GWS linear basis constructions, while

$$\Lambda_1 = t_1 \sum_{r=0}^{\alpha} a_r z^{-r},\ \Psi_1 = t_2 \sum_{r=0}^{\beta} a_r z^{r}, \qquad \Gamma_1 = t_3 \sum_{r=0}^{\gamma} a_r z^{-r},\ \Upsilon_1 = t_4 \sum_{r=0}^{\delta} a_r z^{r}, \tag{11}$$

$$\Lambda_2 = t_5 \sum_{r=0}^{\alpha} a_r z^{-r},\ \Psi_2 = t_6 \sum_{r=0}^{\beta} a_r z^{r}, \qquad \Gamma_2 = t_7 \sum_{r=0}^{\gamma} a_r z^{-r},\ \Upsilon_2 = t_8 \sum_{r=0}^{\delta} a_r z^{r}, \tag{12}$$

where $z = \mathrm{e}^{\mathrm{i}m}$ is the complex modulus. The superscripts $(\alpha, \beta, \gamma, \delta) \geqslant 0$ are integers, to be determined for desired order of accuracy ([6], Appendix A). To maintain time accuracy of the algorithm, one necessary condition for Eqs. (11) and (12) is

$$\Lambda_i + \Psi_i + \Gamma_i + \Upsilon_i = 0; \quad \text{for } i = 1, 2. \tag{13}$$

For Eqs. (9) and (10) the fully discrete weak statement algorithm (4)–(6) assembly at mesh node j with variable $Q_j^n = Q(j\Delta x, t + n\Delta t)$ yields the recursion relation

$$\left(\frac{\Delta x(1-\Gamma_1)}{6\theta\Delta t} - \frac{(1+\Gamma_2)U}{2}\right)_e Q_{j-1} + \left(\frac{\Delta x(4-\Lambda_1-\Upsilon_1)}{6\theta\Delta t} + \frac{(\Lambda_2+\Upsilon_2)U}{2}\right)_e Q_j + \left(\frac{\Delta x(1-\Psi_1)}{6\theta\Delta t} + \frac{(1-\Psi_2)U}{2}\right)_e Q_{j+1} = \text{data from } (n-1) \text{ timestep}. \tag{14}$$

The amplification factor (2) for Eq. (14) is

$$G = \frac{Q_j^{t+\Delta t}}{Q_j^t} = \frac{G_N}{G_D} = \sum_{l=0}^{\infty} A_l m^l, \tag{15}$$

where G_N and G_D can be resolved into spatial $G(x)$ and temporal $G(t)$ components as

$$G_N = G(t) - (1-\theta)CG(x) \text{ and } G_D = G(t) + \theta CG(x), \tag{16}$$

where

$$\begin{aligned} G(t) &= \frac{(1-\Gamma_1)\mathrm{e}^{-\mathrm{i}m} + (4-\Lambda_1-\Upsilon_1) + (1-\Psi_1)\mathrm{e}^{\mathrm{i}m}}{6}, \\ G(x) &= \frac{(1-\Psi_2)\mathrm{e}^{\mathrm{i}m} - (\Lambda_2+\Upsilon_2) - (1+\Gamma_2)\mathrm{e}^{-\mathrm{i}m}}{2}. \end{aligned} \tag{17}$$

Hence, Eq. (16) becomes

$$G_N = \left(\frac{1-\Gamma_1}{6} + (1-\theta)C\frac{1+\Gamma_2}{2}\right)\mathrm{e}^{-\mathrm{i}m} + \frac{4-\Lambda_1-\Upsilon_1}{6} + (1-\theta)\frac{C}{2}(\Lambda_2+\Upsilon_2) + \left(\frac{1-\Psi_1}{6} - (1-\theta)C\frac{1-\Psi_2}{2}\right)\mathrm{e}^{\mathrm{i}m}, \tag{18}$$

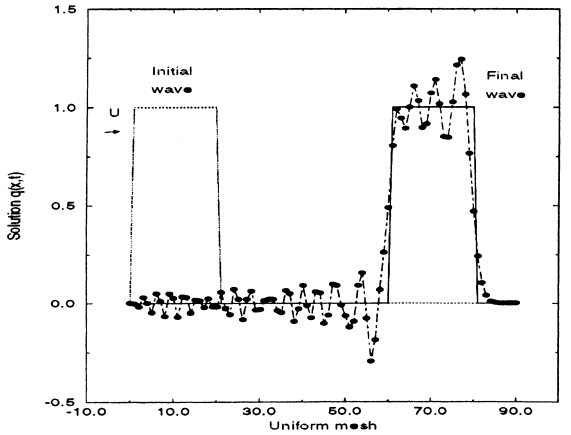
$$G_D = \left(\frac{1-\Gamma_1}{6} - \theta C\frac{1+\Gamma_2}{2}\right)\mathrm{e}^{-\mathrm{i}m} + \frac{4-\Lambda_1-\Upsilon_1}{6} - \theta\frac{C}{2}(\Lambda_2+\Upsilon_2) + \left(\frac{1-\Psi_1}{6} + \theta C\frac{1-\Psi_2}{2}\right)\mathrm{e}^{\mathrm{i}m}.$$

The GMP algorithm amplification factor (15)–(18) may now be expanded in a Laurent series on m. The coefficients of the series may be functionally expressed as

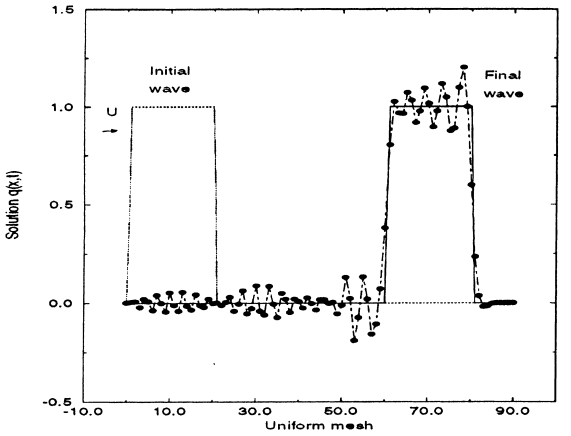
$$A_l = f(C, \theta, t_1, t_2, t_3, t_4, t_5, t_6, t_7, t_8, \alpha, \beta, \gamma, \delta), \tag{19}$$

where l corresponds to the power of m in the Laurent expansion. Comparing the sets a_l of Eq. (3) to A_l of Eq. (15), for a given degree of m a general correlation between C, θ and the elements of [APERT] and [APERX] may be derived that can yield progressively higher order accurate algorithms without adding a

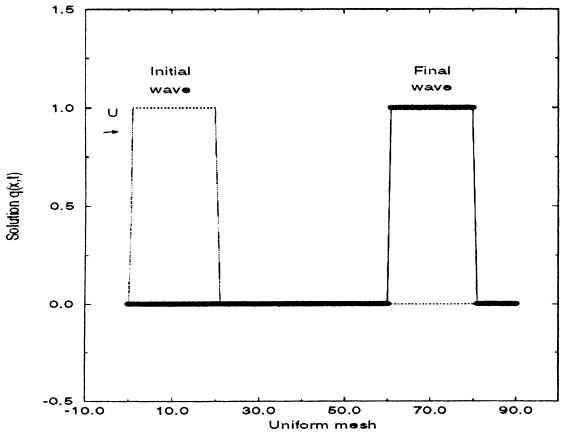
diffusion term to the algorithm. For example, $\alpha = \beta = 0 = \gamma = \delta$ yields a general fourth order accurate algorithm while $\alpha = \beta = 2 = \gamma = \delta$ is at least sixth order accurate which nearly annihilates the phase dispersion error [6], cf. Fig. 1.



(a) GWS solution *second order*



(b) GMP solution *fourth order* ($\beta = \gamma = 0$)



(c) GMP solution *sixth order* ($\beta = \gamma = 2$)

Fig. 1. Comparison square wave solutions for $C = 0.5$ [6].

A simplified example is pertinent to illustrate the process. Selecting

$$\theta = \frac{1}{2},\ \alpha = \beta = \gamma = \delta = 0,\ \text{and}\ t_5 = t_8 = 0 \tag{20}$$

then for the choice

$$t_1 = t_4, t_2 = t_3,\ \text{and}\ t_6 = -t_7 \tag{21}$$

one may produce a fourth order accurate GMP algorithm by satisfying the relationships

$$\begin{aligned} &t_1 + t_2 = 0, \\ &t_6 = -t_7 = \frac{t_2 + t_1}{3} = 0 = t_5 = t_8, \\ &t_1 = t_4 = \frac{3C^2 + (4 - C^2)t_2}{C^2 + 2} = -t_2 = -t_3, \\ &\text{i.e. } t_1 = t_4 = \frac{C^2}{2} = -t_2 = -t_3. \end{aligned} \tag{22}$$

A generally fourth order accurate solution for Eq. (1) may be achieved for the temporal matrix

$$[M]_e = \frac{\Delta x}{6}\begin{bmatrix} 2 - \frac{C^2}{2} & 1 + \frac{C^2}{2} \\ 1 + \frac{C^2}{2} & 2 - \frac{C^2}{2} \end{bmatrix}, \tag{23}$$

while, the convection matrix remains

$$[U]_e = \frac{U}{2}\begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} \tag{24}$$

Using Eq. (22), the solution amplification factor (15) is

$$\begin{aligned} G = 1 - \mathrm{i}(Cm) - \frac{(Cm)^2}{2} + \mathrm{i}\frac{(Cm)^3}{3!} + \frac{(Cm)^4}{4!} - \mathrm{i}\frac{\frac{1}{6}(5C^5 + 5C^3 - 4C)m^5}{5!} - \frac{(5C^4 - 4C^2)m^6}{6!} \\ - i\frac{\frac{1}{12}(35C^7 - 245C^5 + 238C^3 - 40C)m^7}{7!} - \mathrm{O}(m^8). \end{aligned} \tag{25}$$

One can readily see that Eq. (25) matches exactly with Eq. (3) up to the fourth order term ($\mathrm{O}(m^4)$). A similar result may be obtained by using TWS algorithm (see Section 3), which can be made fourth order accurate.

However, as a special case, for $C = 1$, (23) and (24) annihilates the phase dispersion error completely. Selecting $C = 1$ yields $t_1 = t_4 = \frac{1}{2} = -t_2 = -t_3$ and $t_6 = t_8 = t_1 + t_2/3 = 0 = -t_5 = -t_7$, hence

$$\begin{aligned} [M]_e &= \Delta x_e([\mathrm{A200L}] - [\mathrm{APERT}]) = \frac{\Delta x_e}{4}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \\ [U]_e &= U([\mathrm{A201L}] - [\mathrm{APERX}]) = \frac{U}{2}\begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} \end{aligned} \tag{26}$$

for which the amplification factor of the approximation solution for Eq. (1), in terms of wave number m, is exact (matched) with the analytical solution amplification factor to *umpteenth* order.

For another example, selecting $C = 2$ yields

$$\begin{aligned} [M]_e &= \frac{\Delta x_e}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \\ [U]_e &= \frac{U}{2}\begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} \end{aligned} \tag{27}$$

Here, again, the solution amplification factor, in terms of wave number m, is exact (matched) to *umpteenth* order with the analytical solution amplification factor (3). However, in this case, one may not obtain the exact solution numerically using Eq. (27). In general, a von Neumann frequency analysis is necessary but

not sufficient to guarantee the approximate solution accuracy. Specifically, matching the coefficients of equal powers of m in Eqs. (3) and (15) only guarantees that the ratio $C^h/C = 1$, but does not guarantee the phase velocity relationship $U^h = U$.

A specific order of solution accuracy, e.g. *tenth order*, can be achieved by selecting the summation limits $\alpha, \beta, \gamma, \delta$ in Eqs. (11) and (12) for [APERT] and [APERX]. The corresponding coefficients t_1–t_8 in Eqs. (11) and (12) can then be determined. For example, selecting $\beta = \gamma = \alpha = \delta = 2$ guarantees a *sixth order* accurate solution for *any* a_r, $0 \leqslant r \leqslant \alpha, \beta, \gamma, \delta$.

Although the GMP algorithm needs only two element support for each node, i.e. the equation for Q_j involves Q_{j-1} and Q_{j+1} only, the procedure Eqs. (9) and (10) results can be compared directly with compact finite difference schemes, cf. Ref. [3]. However, the theory and implementation of GMP is much simpler. Also note that the GMP assembly matrices in Eqs. (23)–(26) retain the efficiency of a linear basis (or centered FD) algorithm form.

3. Combining GMP with TWS class of algorithm

The Taylor class of algorithms has been widely verified and documented in the literature, cf., [1,7–13]. The Taylor– Galerkin algorithm [9,12] couples the Taylor time series with fourth order accurate spatial Galerkin approximation. The Taylor-least-square method [11] utilizes the least square method of [10] with the high-order time approximation of Taylor series. Later, the TWS algorithm [1] evolved from the Taylor–Galerkin method with some optimization of parameters to reduce dispersion error in linear basis finite elements. These methods have been successfully implemented for solving the multidimensional form of Eq. (1). In this section, the combination TWS–GMP algorithm is developed to extract the multidimensional capability of Galerkin spatial discretization of TWS and the high order accuracy of GMP implicit time-step algorithm in order to produce high order accurate fully discrete method for the numerical solution of the first order hyperbolic and advection–diffusion type problems.

Assuming sufficient continuity in the solution, the forward time semi-discretized Taylor series is

$$q^{n+\vartheta} = q^n + \vartheta\Delta t\frac{\partial q^n}{\partial t} + \frac{\vartheta^2\Delta t^2}{2}\frac{\partial^2 q^n}{\partial t^2} + \frac{\vartheta^3\Delta t^3}{6}\frac{\partial^3 q^n}{\partial t^3} + \frac{\vartheta^4\Delta t^4}{24}\frac{\partial^4 q^n}{\partial t^4} + \frac{\vartheta^5\Delta t^5}{120}\frac{\partial^5 q^n}{\partial t^5} + \mathrm{O}(\Delta t^6), \tag{28}$$

where ϑ is an upwind level. The corresponding backward time semi-discrete Taylor series is

$$q^{n+(1-\vartheta)} = q^{n+1} - \vartheta\Delta t\frac{\partial q^{n+1}}{\partial t} + \frac{\vartheta^2\Delta t^2}{2}\frac{\partial^2 q^{n+1}}{\partial t^2} - \frac{\vartheta^3\Delta t^3}{6}\frac{\partial^3 q^{n+1}}{\partial t^3} + \frac{\vartheta^4\Delta t^4}{24}\frac{\partial^4 q^{n+1}}{\partial t^4} - \frac{\vartheta^5\Delta t^5}{120}\frac{\partial^5 q^{n+1}}{\partial t^5} + \mathrm{O}(\Delta t^6). \tag{29}$$

Using Eq. (28), for $\vartheta = 1/2$ and 1, [8] derived

$$q^{n+1} - q^n - \Delta t\frac{\partial q^n}{\partial t} = \frac{\Delta t^2}{6}\frac{\partial^2 q^n}{\partial t^2} - \frac{\Delta t^4}{144}\frac{\partial^4 q^n}{\partial t^4} - \frac{\Delta t^5}{480}\frac{\partial^5 q^n}{\partial t^5} + \mathrm{O}(\Delta t^6). \tag{30}$$

Similarly, for $\vartheta = 1/3$ and $2/3$ in Eq. (28)

$$q^{n+1} - q^n - \Delta t\frac{\partial q^n}{\partial t} = \frac{\Delta t^2}{9}\frac{\partial^2 q^n}{\partial t^2} - \frac{\Delta t^4}{486}\frac{\partial^4 q^n}{\partial t^4} - \frac{\Delta t^5}{2430}\frac{\partial^5 q^n}{\partial t^5} + \mathrm{O}(\Delta t^6). \tag{31}$$

Finally, a weighted combination of Eqs. (30) and (31) yields

$$q^{n+1} - q^n - \Delta t\frac{\partial q^n}{\partial t} = \frac{5\Delta t^2}{57}\frac{\partial^2 q^n}{\partial t^2} + \frac{\Delta t^5}{10}\frac{\partial^5 q^n}{\partial t^5} + \mathrm{O}(\Delta t^6). \tag{32}$$

Similarly, using Eq. (29), for $\vartheta = 1/2$ and 1, one may derive

$$q^{n+1} - q^n - \Delta t\frac{\partial q^{n+1}}{\partial t} = -\frac{\Delta t^2}{6}\frac{\partial^2 q^{n+1}}{\partial t^2} + \frac{\Delta t^4}{144}\frac{\partial^4 q^{n+1}}{\partial t^4} - \frac{\Delta t^5}{480}\frac{\partial^5 q^{n+1}}{\partial t^5} + \mathrm{O}(\Delta t^6). \tag{33}$$

Again, for $\vartheta = 1/3$ and $2/3$ in Eq. (29), we find

$$q^{n+1} - q^n - \Delta t \frac{\partial q^{n+1}}{\partial t} = -\frac{\Delta t^2}{9}\frac{\partial^2 q^{n+1}}{\partial t^2} + \frac{\Delta t^4}{486}\frac{\partial^4 q^{n+1}}{\partial t^4} - \frac{\Delta t^5}{2430}\frac{\partial^5 q^{n+1}}{\partial t^5} + \mathrm{O}(\Delta t^6). \tag{34}$$

and a weighted combination of Eqs. (33) and (34) yields

$$q^{n+1} - q^n - \Delta t \frac{\partial q^{n+1}}{\partial t} = -\frac{5\Delta t^2}{57}\frac{\partial^2 q^{n+1}}{\partial t^2} - \frac{\Delta t^5}{10}\frac{\partial^5 q^{n+1}}{\partial t^5} + \mathrm{O}(\Delta t^6). \tag{35}$$

Finally, multiplying Eq. (32) by $(1-\theta)$ and Eq. (35) by θ and then adding them together (since $q^{n+\theta} \approx \theta q^{n+1} + (1-\theta)q^n$), we get

$$\begin{aligned} &q^{n+1} - q^n - \Delta t\left(\theta\frac{\partial q^{n+1}}{\partial t} + (1-\theta)\frac{\partial q^n}{\partial t}\right) \\ &\quad = -\frac{5\Delta t^2}{57}\left(\theta\frac{\partial^2 q^{n+1}}{\partial t^2} - (1-\theta)\frac{\partial^2 q^n}{\partial t^2}\right) - \frac{\Delta t^5}{10}\left(\theta\frac{\partial^5 q^{n+1}}{\partial t^5} - (1-\theta)\frac{\partial^5 q^n}{\partial t^5}\right) + \mathrm{O}(\Delta t^6). \end{aligned} \tag{36}$$

For the 1-D form of Eq. (1), $\mathscr{L}(q) = \partial q/\partial t + (U - \epsilon(\partial\ /\partial x))\partial q/\partial x$, one may write

$$\frac{\partial q}{\partial t} = -\left(U - \epsilon\frac{\partial}{\partial x}\right)\frac{\partial q}{\partial x} \tag{37}$$

and

$$\frac{\partial^2 q}{\partial t^2} = \frac{\partial}{\partial x}\left(U - \epsilon\frac{\partial}{\partial x}\right)\left(U - \epsilon\frac{\partial}{\partial x}\right)\frac{\partial q}{\partial x}. \tag{38}$$

Hence, from Eq. (36) via Eqs. (37) and (38)

$$\begin{aligned} &q^{n+1} - q^n - \Delta t\left(U - \epsilon\frac{\partial}{\partial x}\right)\frac{\partial}{\partial x}\left(\theta q^{n+1} + (1-\theta)q^n\right) \\ &\quad = -\frac{5\Delta t^2}{57}\left(U^2 - 2U\epsilon\frac{\partial}{\partial x}\right)\frac{\partial^2}{\partial x^2}\left(\theta q^{n+1} - (1-\theta)q^n\right) + \mathrm{O}(\Delta t^5, \epsilon^2). \end{aligned} \tag{39}$$

Note that Eq. (39) is *naturally* $\mathrm{O}(\Delta t^5, \epsilon^2)$, i.e. *fourth-order* accurate in time.

Again, for trapezoidal condition ($\theta = 1/2$)

$$q^{n+1} - q^n - \frac{\Delta t}{2}\left(U - \epsilon\frac{\partial}{\partial x}\right)\frac{\partial}{\partial x}\left(q^{n+1} + q^n\right) + \frac{\Delta t^2}{12}\left(U^2 - 2U\epsilon\frac{\partial}{\partial x}\right)\frac{\partial^2}{\partial x^2}\left(q^{n+1} - q^n\right) = \mathrm{O}(\Delta t^4, \epsilon^2). \tag{40}$$

Defining the global term integrals as

$$\begin{aligned} &\mathbf{M} \equiv \int_\Omega \phi_j \phi_i \,\mathrm{d}\Omega, \qquad \mathbf{U} \equiv \int_\Omega \phi_j \phi_{i_x} \,\mathrm{d}\Omega, \\ &\mathbf{D} \equiv \int_\Omega \phi_{j_x} \phi_{i_x} \,\mathrm{d}\Omega, \qquad \mathbf{E} \equiv \int_\Omega \phi_{j_x\ x} \phi_{i_x} \,\mathrm{d}\Omega \end{aligned} \tag{41}$$

Eq. (39) may be written in a general form as

$$\begin{aligned} &\left(\mathbf{M} + (\theta - \hat{\alpha})(C\Delta x)\mathbf{U} + (\hat{\gamma} + \hat{\beta}\theta)(C\Delta x)^2\mathbf{D} + \hat{\mu}\theta(C\Delta x)^3\mathbf{E}\right)Q^{n+1} \\ &\quad = \left(\mathbf{M} - (1 - \theta + \hat{\alpha})(C\Delta x)\mathbf{U} + \hat{\gamma} - (1-\theta)\hat{\beta})(C\Delta x)^2\mathbf{D} - \hat{\mu}(1-\theta)(C\Delta x)^3\mathbf{E}\right)Q^n, \end{aligned} \tag{42}$$

where for Eq. (40), $\hat{\alpha} = 0$, $\hat{\beta} = \epsilon/(U^2\Delta t) = \varepsilon$ (non-dimensional diffusion coefficient), $\hat{\gamma} = -1/12$ and $\hat{\mu} = \pm\varepsilon/3$. In Ref. [12], a similar Bubnov–Galerkin scheme with α and β as free perturbation parameters is proposed.

In comparison the corresponding GMP algorithm general form can be written as [6]

$$\Big((\mathbf{M}-\mathbf{M}^{\varepsilon})+\theta\Big[(C\Delta x)(\mathbf{U}-\mathbf{U}^{\varepsilon})\ +(C\Delta x)^2(\mathbf{D}-\mathbf{D}^{\varepsilon})+(C\Delta x)^3(\mathbf{E}-\mathbf{E}^{\varepsilon})\Big]\Big)Q^{n+1}$$
$$=\Big((\mathbf{M}-\mathbf{M}^{\varepsilon})-(1-\theta)\Big[(C\Delta x)(\mathbf{U}-\mathbf{U}^{\varepsilon})-(C\Delta x)^2(\mathbf{D}-\mathbf{D}^{\varepsilon})-(C\Delta x)^3(\mathbf{E}-\mathbf{E}^{\varepsilon})\Big]\Big)Q^{n}, \tag{43}$$

where upon full discretization $\mathbf{M}\Rightarrow[M]_e$, and $\mathbf{M}^{\varepsilon}\Rightarrow[\mathrm{APERT}]_e$; $\mathbf{U}\Rightarrow[U]_e$, and $\mathbf{U}^{\varepsilon}\Rightarrow[\mathrm{APERX}]$, and so on. One may see that for no physical diffusion, i.e. $\epsilon=0$, Eq. (42) is identical with GMP algorithm Eq. (7) and (8) for $[\mathrm{APERT}]_e=0$ and

$$[\mathrm{APERX}]_e C\Delta x\Big(\theta\{Q\}^{n+1}+(1-\theta)\{Q\}^{n}\Big)=\alpha[U](Q^{n+1}-Q^{n}). \tag{44}$$

Here, the general form of amplification factor (2) for Eq. (43) is

$$G=\frac{Q^{n+1}}{Q^{n}}=\frac{G(t)-(1-\theta)[CG_u(x)-C^2G_d(x)-C^3G_e(x)]}{G(t)+\theta[CG_u(x)+C^2G_d(x)+C^3G_e(x)]}. \tag{45}$$

Here the spatial $G(x)$ and temporal $G(t)$ components of Eq. (16) can be written as

$$\begin{aligned}G(t)&=\mathbf{M}-\mathbf{M}^{\varepsilon},\\ G_u(x)&=\Delta x(\mathbf{U}-\mathbf{U}^{\varepsilon}),\\ G_d(x)&=(\Delta x)^2(\mathbf{D}-\mathbf{D}^{\varepsilon}),\\ G_e(x)&=(\Delta x)^3(\mathbf{E}-\mathbf{E}^{\varepsilon}).\end{aligned} \tag{46}$$

Note that the GMP–TWS algorithm amplification factor (45) is unconditionally stable for all C.

4. Discussion and results

4.1. Verification smooth and non-smooth wave convection, $C\leqslant 1$

An isolated energy packet is a standard verification problem that has been studied for one dimensional pure convection wave propagation by Refs. [1,5–13] using FE, finite volume (FV), and various finite difference (FD) algorithms. The analytical solution $q(x,t)$ to Eq. (1) , for $f(u)=u$ and $s=0$, is exact preservation of the initial condition $q(x,t=t_0)$ as it is convected parallel to x on Ω over $n\Delta t$. Computational result herein verify theory and summarize performance for the traveling wave propagation verification problem, for a range of Courant numbers with a cluster of four different initial condition sets including a step function, a gaussian wave, a cosine hill and a sharp cone of different initial wavelengths, [14]. The non-dissipative trapezoidal rule ($\theta=0.5$) time integration algorithm is used for all verification problems.

Fig. 2 documents the initial condition and the computational solutions of the four wave cluster convection using GWS, TWS, FV and GMP algorithms. Solution data are compared for Courant number $C=1$ after 50 s. The GWS solution is non-dissipative and dispersive, as theoretically predicted, with trailing oscillatory maxima about 40% and with peak level reduced (via distortion) by almost 50%, Fig. 2a. Similar dispersion error wave is observed in Fig. 2c for FV algorithm. Corresponding TWS solution, Fig. 2b, for $\hat{\beta}=0.9$ is less dispersive but highly distorted by numerical disspation. The comparative GMP algorithm (26) $C=1$ solution for $\beta=\gamma=0$ is dispersion free and nodally exact to within round-off error (order 10^{-16}), Fig. 2d.

In a theoretical analysis [6] proved that only for $C=0,1$ and 2 one may match the numerical and analytical solution to Eq. (1) identically. Hence, a non-unit Courant number, say $C=0.4$, solution will be the test. Note that choice of $C=0.4$ is arbitrary. The GMP–TWS algorithm of Eq. (43) is guaranteed for solution stability and improved accuracy for all C (see Section 3). For the specification of $C=0.4$, propagation of the wave cluster for 50 seconds reduces the leading (negative) extremum of the GWS solution by nearly 20% and trailing dispersion error dominates the entire solution, Fig. 3a. Artificial diffusion generally smoothes out these "wrinkles". However, determining the appropriate coefficient $\hat{\beta}$ for damping

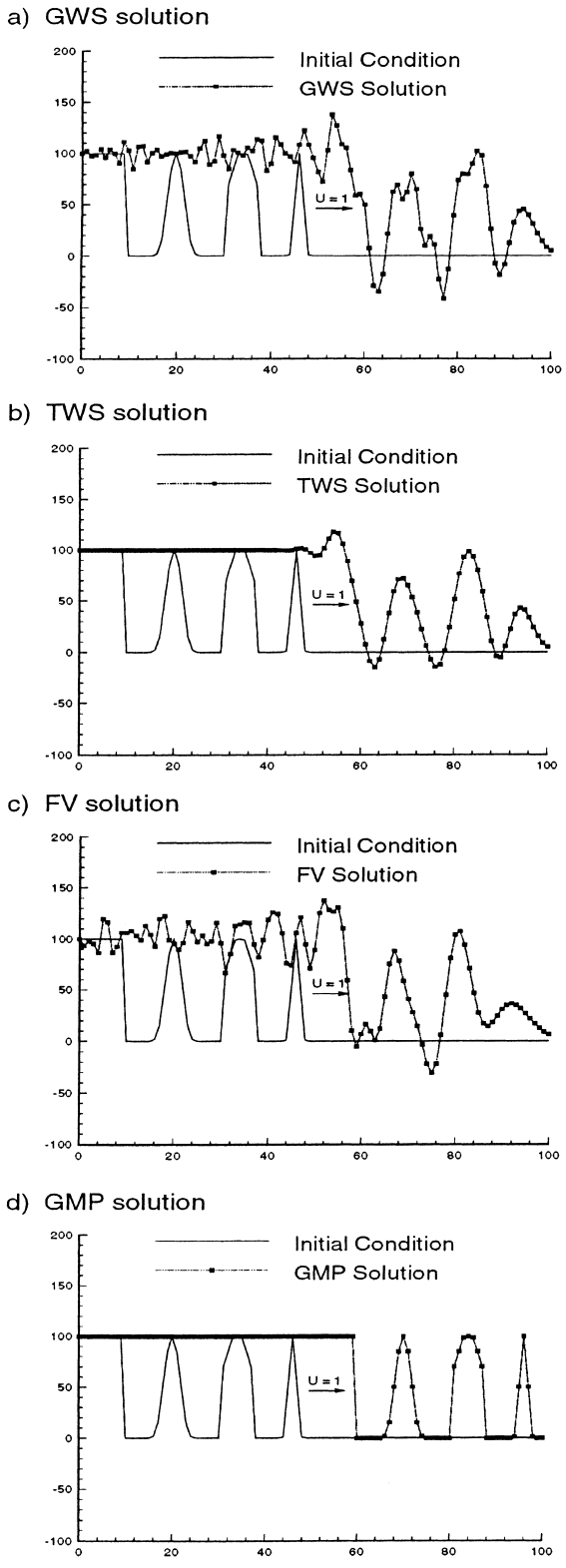


Fig. 2. Wave group propagation at $C = 1.0$.

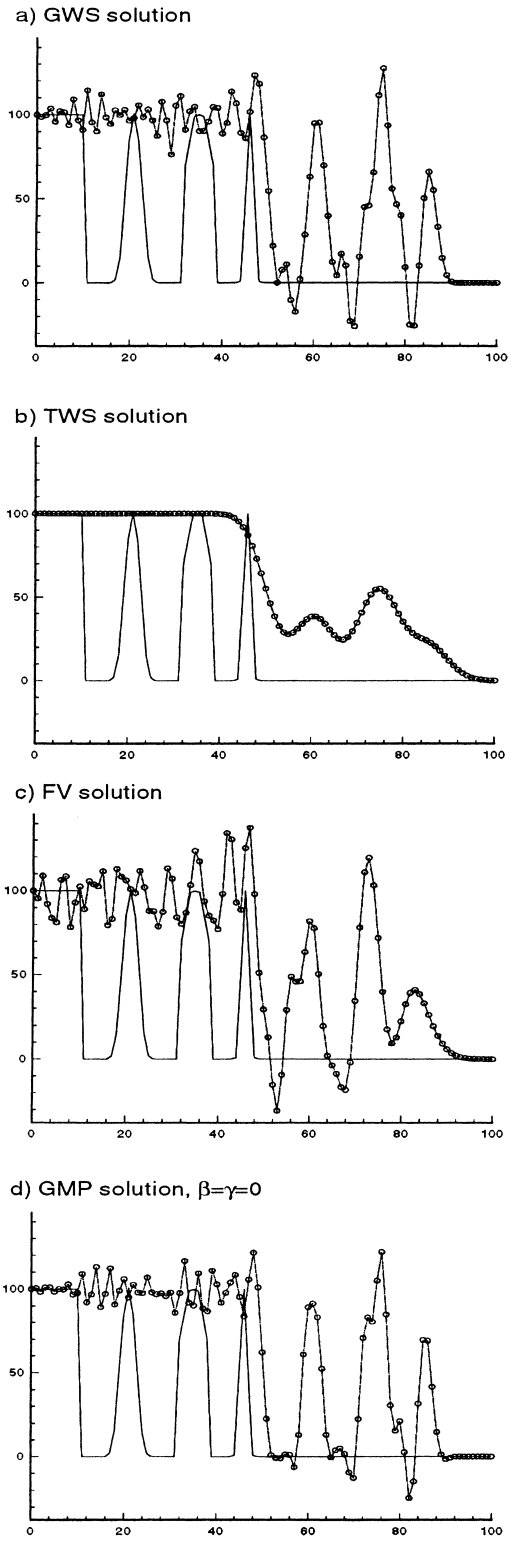


Fig. 3. Wave group propagation at $C = 0.4$.

mechanism is not easy and any particular choice of $\hat{\beta}$ almost always either retains some dispersion error wrinkles or dissipates the solution excessively distorting its analytical characteristics.

For example, selecting $\hat{\beta} = 0.5$, TWS solution in Fig. 3b is totally non-dispersive, although excess diffusion nearly annihilates the convected wave peaks. Corresponding FV solution, Fig. 3c, has more trailing dispersion error than the GWS solution, Fig. 3a, while the leading oscillations remain relatively unchanged. For this non-unit Courant number, the *fourth order accurate* ($\beta = \gamma = 0$) GMP algorithm (23), Fig. 3d, reduces large wavelength leading edge oscillations of the companion GWS or FV solutions by ~50%. However, the solution still suffers from a non-dissipative dispersion error wave.

Examples of very high order accurate GMP options (e.g., at least *sixth* order accurate with $\alpha, \beta, \gamma, \delta \geqslant 2$) for this problem class are documented in [6,7] that yields a non-dissipative dispersion error-free solution, cf. Fig. 1c. However, deriving the problem specific temporal and convective matrices for sixth order accuracy is computationally complicated and requires symbolic logic expertise. In addition, very high order accurate algorithms are generally prone to solution instability. In this paper a different approach is introduced. The idea is to simultaneously reduce the dispersive and dissipative error to an *optimum* level by using TWS $\hat{\beta} > 0$ artificial diffusion matrix along with the GMP fourth order accurate Eq. (23) matrices. This combination (GMP–TWS) guarantees minimal artificial diffusion and a good solution stability.

Fig. 4 documents the comparison $C = 0.4$ TWS and GMP–TWS solutions after 50 seconds. In Fig. 4a, the TWS solution for $\hat{\beta} = 0.5$ has no dispersion error although the solution is nearly "flat" and the information peaks have dissipated by almost 70%. The step function is also lost. A smaller value of $\hat{\beta}$ may bring back the peaks at the expense of dispersion error waves. Conversely, for $\beta = \gamma = 0, \hat{\beta} = 0.2$ GMP–TWS algorithm solution is nearly dispersion-error free, Fig. 4b. The essential character of the wave cluster is also retained. In particular, note that the step function is fully preserved after 50 s.

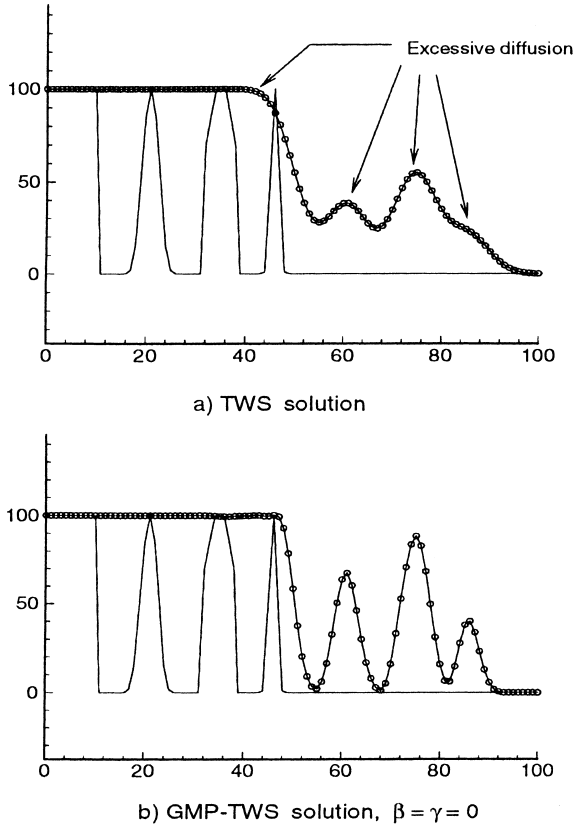


Fig. 4. Comparison TWS and GMP–TWS solution, $C = 0.4$.

5. Conclusions

A weak statement perturbation technique based on Fourier modal analysis of the approximation solution amplification factor has been developed for generating progressively higher order accurate CFD algorithm constructions for non-diffusive (pure convection) applications. It exhibits the efficiency of a strictly linear basis FE GWS (or centered FD) algorithm. Using the TWS numerical diffusion along with analytical fourth order accurate GMP matrix is a viable option to improve the solution resolution at minimal computational cost. The multidimensional theoretical analysis is necessary for effective practical application of GMP–TWS algorithm.

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