XVIII International Conference on Water Resources
CMWR 2010
J. Carrera (Ed)

A GENERALIZED FLUX CORRECTION FOR CONTINUOUS-FEM IN ADVECTIVE TRANSPORT

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Key words: Continuous Galerkin finite elements, Positive definite algorithm

Summary. This work presents a sign–preserving continuous finite element model (FEM) for advection, incorporating an enhanced flux corrected transport method (FCT) with a high order solution founded in the characteristic based (CB) FEM. The method extends the inherent correction process of the FCT by assuming a general predictor–type positive solution that allows the inclusion of precedent discarded contributions.

1 INTRODUCTION

Sign–preservation is essential for an algorithm to avoid unphysical computed values of a positive definite property transported by a fluid flow. In Ref. 6 we introduced a sign–preserving finite element model for advection problems (NFEM, in short form), retaining the *continuous* nature of the FEM. The method integrates the flux corrected transport technique (FCT) [1,4,10,11] with the (high order) characteristic based (CB) FEM [7,12,13].

This work proposes an extension of the correction procedure, allowing the successive reduction of the rejected element contributions. To achieve these reductions, we extend the NFEM to include a general predictor (positive preserving) solution. The format of the modified method has four leading tasks, (a) Computation of a high order solution (HO) by the CB-FEM, (b) Computation of a predictor sign-preserving solution, (c) Calculation of the *anti-diffusive* contributions by limiting the difference between contributions of method (a) and method (b), and (d) Computation of final, sign-preserving, corrected solution, by adding the limited contributions to the predictor solution.

As a first natural approach, an iterative procedure using previous corrected solution as predictor solution for the step (b) is tested, showing a considerable improvement after few loops. A pioneering use of this idea in FD can be found in Ref. 8, although the iterative process is close to the iterative–FEM presented by Kuzmin and Moller [3], differing mainly in the initial predictor method. The NFEM uses a low order solution of upwind type, independent of the CBS-FEM algorithm. Its (nearly) minimum diffusion to assure positivity helps to a faster reach of the desired tolerance of discarded contributions.

2 THE NON–OSCILLATORY FEM MODEL

2.1 Model problem

The model problem is the advective–source transport equation

$$\frac{\partial B}{\partial t} + \nabla \cdot (\mathbf{u}B) + \mathcal{R} = 0 \;\text{ in } \Omega \;, t \in [t_0, T] \;, \tag{1}$$

with boundary conditions

$$\begin{aligned} B &= \overline{B}(X,t) \;\text{ on } \Gamma_B^- \quad \text{(a)} \;, \\ B\mathbf{u}\cdot\mathbf{n} &= \overline{\mathbf{q}}_B(X,t)\cdot\mathbf{n} \;\text{ on } \Gamma_q^- \quad \text{(b)} \;, \\ \Gamma^- = \Gamma_B^- \cup \Gamma_q^- \;, &\quad \Gamma^- = \{X \in \Gamma : (\mathbf{u}\cdot\mathbf{n}) \leq 0\} \end{aligned} \tag{2}$$

and initial conditions

$$B(X, t_0) = \overline{B}_0(X) \;\text{ in } \Omega \;, \tag{3}$$

where B is a scalar transported by the advective velocity field $\mathbf{u}$, $\mathcal{R} = \mathcal{R}(B, X, t)$ is a source, $(X{=}(x_l), l{=}1, d)$, Ω is a domain in $\mathbf{R}^d$ bounded by $\Gamma = \Gamma^- + \Gamma^+$, d is the number of space dimension, $\overline{B}$, $\overline{B}_0$ and $\overline{\mathbf{q}}_B$ are known (the latter a vector) functions, and $[t_0, T]$ is the time interval. The inflow boundary is denoted by Γ^- while Γ_q^- includes slip condition if suitable, $\Gamma^+ = \{X \in \Gamma : (\mathbf{u}\cdot\mathbf{n}) > 0\}$ is the outflow boundary and $\mathbf{n}$ is the outward unit normal to the boundary.

2.2 The general correction method

We start the formulation by introducing a high order continuous finite element method for the model problem. The method written in matrix form is

$$\frac{1}{\Delta t}\mathbf{M}_c \Delta\mathbf{B} = \mathbf{R}_H \;, \tag{4}$$

where $\Delta t = t^{n+1} - t^n$ is the time step, $\mathbf{B}$ represents the high order solution, $\Delta\mathbf{B} = \mathbf{B}^{n+1} - \mathbf{B}^n$ and superscripts indicate time level. $\mathbf{R}_H$ is the right hand side for the high order algorithm and $\mathbf{M}_c$ is the consistent mass matrix. $\mathbf{B}^n$ is such that $B_i^n \geq 0$ for all node i. Next, we introduce a predictor–type monotonic (or at least definite positive) method. In matrix form,

$$\frac{1}{\Delta t}\mathbf{M}'_L \Delta\mathbf{b} = \mathbf{R}_L \;, \tag{5}$$

where $\mathbf{b}$ is the corresponding unknown and $\Delta\mathbf{b} = \mathbf{b}^{n+1} - \mathbf{B}^n$. $\mathbf{R}_L$ is the right hand side computed for the predictor algorithm and $\mathbf{M}'_L$ is a conservative diagonal matrix that ensures sign preservation. Now, Equation (4) is written as

$$\frac{1}{\Delta t}\mathbf{M}'_L \Delta\mathbf{B} = \mathbf{R}_H + \frac{1}{\Delta t}\left(\mathbf{M}'_L - \mathbf{M}_c\right)\Delta\mathbf{B} \;. \tag{6}$$

By subtracting Equation (5) from Equation (6) and by replacing Eqs. (5) and (4) on the rhs, an alternate form of value in the implementation is the identity

$$\mathbf{B}^{n+1} = \mathbf{b}^{n+1} + \sum_{j=1}^{E} (\mathbf{M}'_L)^{-1} \{\mathbf{M}'_L(\mathbf{B}^{n+1} - \mathbf{b}^{n+1})\}_j \ . \tag{7}$$

The finite element method subdivides the domain Ω by E elements Ω_j, $(j = 1, E)$, such that $\Omega = \bigcup \Omega_j$. In the identity (7), the assembling of the product $\{\mathbf{M}'_L(\mathbf{B}^{n+1} - \mathbf{b}^{n+1})\}_j$ for each j element is explicitly written, and extended over the total number of elements.

The HO–FEM solution (Equation (7)) is written for a node i as

$$B_i^{n+1} = b_i^{n+1} + \sum_{j=1}^{e} A_j = b_i^{n+1} + \sum_{j=1}^{e} (A_j^H - A_j^P) \ . \tag{8}$$

where B_i at time $(n+1)\Delta t$ results from updating the predictor solution at time $(n+1)\Delta t$ by the sum of A_j, the *element contributions* to node i extended over e, the total number of elements j surrounding i. The element contribution is the difference between that obtained by the HO solution, A^H, and that obtained by the predictor scheme, A^P. The monotonicity– (or at least sign–)preservation for the predictor method, along the lines of Smolarkiewicz and Grabowski [9] for monotone FD schemes, is formally imposed by bounding the new solution b_i^{n+1} as

$$B_i^{min} \leq b_i^{n+1} \leq B_i^{max} \tag{9}$$

such that $b_i^{n+1} \geq 0$ for all i. The procedure concludes by computing the enhanced HO solution $\tilde{B}_i$ as

$$\tilde{B}_i^{n+1} = b_i^{n+1} + \sum_{j=1}^{e} \tilde{A}_j = b_i^{n+1} + \sum_{j=1}^{e} \{cA\}_j \ , \tag{10}$$

where the c_j's are elementwise correcting functions depending on nodal HO solution, nodal predictor solution and element contribution to the node. The implementation of the correction procedure is analogous to the FCT method, and can be established by considering identity (7). Therefore, the contribution of element j is $A_j = (\mathbf{M}'_L)^{-1}\{\mathbf{M}'_L(\mathbf{B}^{n+1} - \mathbf{b}^{n+1})\}_j$ (see details in Ref. 6). The simplest predictor solution is a low order monotonic solution (LO). The FEM–FCT method [4] employs the Taylor–Galerkin finite element method [2,5] as high order option and the Taylor–Galerkin algorithm with lumped mass matrix plus added diffusion as the corresponding low order scheme. LO scheme of the FEM–FCT reaches positivity with supplementary diffusion of the type $\alpha(\mathbf{M}_c - \mathbf{M}_L)\mathbf{B}^n$, where α is a diffusion coefficient to be specified. Instead, the NFEM is designed by the combination of a characteristic based high order method and a low order method of upwind type as predictor solution. The high order solution is an abridged version of the complete characteristic based finite element method formulated in Ref. 6.

3 AN ITERATIVE CORRECTION

To illustrate the application of the proposed methodology, we present in this section an iterative option. This option generalize that presented by Schar and Smolarkiewicz [8] by updating bounds every iteration. We introduce the nodal enhanced solution $\tilde{B}_i^{(p)}$, at step (p) of an iteration process and at time t^{n+1}, such that

$$\tilde{B}_i^{(p)} = b_i^{(p)} + \sum_{j=1}^{e} \{c^{(p)} A^{(p)}\}_j \ . \tag{11}$$

The predictor solution is defined as that computed by the correction method in the preceding $(p-1)$ step. Hence, $b_i^{(p)} := \tilde{B}_i^{(p-1)}$. The iterative method (11), taking into account the identity (7), is

$$\tilde{B}_i^{(p)} = b_i^{(p)} + \sum_{j=1}^{e} c_j^{(p)} (\mathbf{M}'_L)^{-1} \{(\mathbf{M}'_L)(\mathbf{B}^{(p)} - \mathbf{b}^{(p)})\}_j \ , \tag{12}$$

where $\mathbf{B}^{(p)}$ is the high order solution for iteration (p). For a node i, the HO solution is

$$B_i^{(p)} = b_i^{(p)} + \sum_{j=1}^{e} A_j^{(p)} \ . \tag{13}$$

The $A_j^{(p)}$ are the contributions *rejected* in the $p-1$ step,

$$\sum_{j=1}^{e} A_j^{(p)} = \sum_{j=1}^{e} \{(1 - c^{(p-1)})\, A^{(p-1)}\}_j \ . \tag{14}$$

Solution computed by Equation (13) does not preserve positivity, whereas the method (12) conserves sign.

3.1 Implementation of the procedure

We construct the iteration loop by using the NFEM for the zero iteration. In this step, predictor corresponds to the LO algorithm.

- *Zero iteration calculation*, $b_i^{(0)}$: Predictor solution by a LO method.
- *Initialization* ($b_i^{(1)} := \tilde{B}_i^{(0)}$).

Now, each iteration has three basic loops. For the iteration (p),
For p=1, iter;   *iter*: number of iterations,

- *Loop over elements*

1. Computation of new bounds (Zalezak criteria [11])

$$B_i^{min} = \min_{j=1,e} \left(B_i^n, \tilde{B}_i^{(p-1)}, B_k^n, \tilde{B}_k^{(p-1)} \right), \quad \forall \text{ (nodes } k \neq i) \in j \quad ,$$

$$B_i^{max} = \max_{j=1,e} \left(B_i^n, \tilde{B}_i^{(p-1)}, B_k^n, \tilde{B}_k^{(p-1)} \right), \quad \forall \text{ (nodes } k \neq i) \in j \quad .$$

2. Computation of rejected fluxes, storing at nodes

$$\sum_{j=1}^{e} A_j^{(p)+} = \sum_{j=1}^{e} \{(1-c)A\}_j^{(p-1)+} \quad ; \sum_{j=1}^{e} \mid A_j^{(p)-} \mid = \sum_{j=1}^{e} \{(1-c) \mid A \mid\}_j^{(p-1)-}$$

(note that $A_j^{(p-1)+/-} = (\mathbf{M}'_L)^{-1}\{\mathbf{M}'_L(\tilde{\mathbf{B}}^{(p-1)} - \mathbf{b}^{(p-1)})\}_j$).

- *Loop over nodes*

1. Updating high order solution by using rejected fluxes stored at nodes

$$B_i^{(p)} = \tilde{B}_i^{(p-1)} + \sum_{j=1}^{e} A_j^{(p)+} - \sum_{j=1}^{e} \mid A_j^{(p)-} \mid$$

2. Nodal correcting functions c_i

$$c_i^{(p)+} \leq \min \left(1, \frac{B_i^{max} - \tilde{B}_i^{(p-1)}}{\left(\sum_{j=1}^{e} A_j^{(p)+} \right) + \mu} \right) \quad ; c_i^{(p)-} \leq \min \left(1, \frac{\tilde{B}_i^{(p-1)} - B_i^{min}}{\left(\sum_{j=1}^{e} \mid A_j^{(p)-} \mid \right) + \mu} \right)$$

- *Loop over elements*

1. Computation of elementwise correcting functions c_j

$$c_j^{(p)+} = \min(c_k^{(p)+}), \quad c_j^{(p)-} = \min(c_k^{(p)-}) \quad \forall \text{ nodes } k \in j \ ,$$

2. Computation of (p) corrected solution

$$\tilde{B}_i^{(p)} = \tilde{B}_i^{(p-1)} + \sum_{j=1}^{e} (\mathbf{M}'_L)^{-1} \{ c^{(p)} \mathbf{M}'_L (\mathbf{B}^{(p)} - \tilde{\mathbf{B}}^{(p-1)}) \}_j \qquad (15)$$

End iter (p).

3.2 A long term smooth solution

FCT method can produce distorted solutions for advection of certain smooth profiles, as the case discussed here (along the lines of that performed in Ref. 8). The initial condition of the problem is given by a sine function of wavelength λ. This scalar field is transported a distance of 100λ. The time step is 0.4 s and final time corresponds to $12500\Delta t$ (5000 s). The advection velocity field is constant (1 m/s), while average number of nodes per wavelength is 50. The finite element grid has 10201 nodes and 20000 triangular elements of base unity and height unity in a $[0,100]\times[0,100]$ region. To simulate the propagation of the profile, periodic conditions were imposed on left and right boundaries. Results in Fig. 1 correspond to the CB algorithm, NFEM and the iterative NFEM for

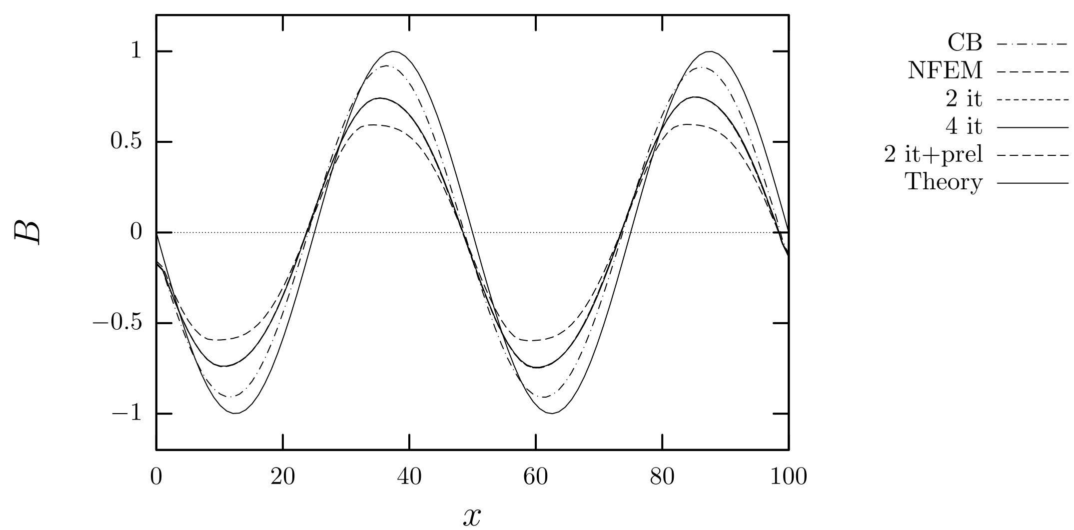

Figure 1: Sine wave experiment. Theoretical and numerical results for the CB–FEM, NFEM, iterative NFEM (2 iterations), iterative NFEM (4 iterations) and iterative NFEM with prelimiter (2 iterations). $t = 12500\Delta t$; $\Delta t = 0.4$; $\Delta x = 1$.

2 and 4 iterations, superimposed on the analytical solution. Pathology of original flux correction technique is seen in the asymmetrical results of NFEM, as well as a diffusion error at the peak of around 40%, while this error for CB–FEM is of around 10%. The refined amount of rejected contributions given by the iterative method permits a drastic reduction of diffusion error at the peak (around 25%), a decrease of L_∞ error and L_2 error, as well as a nearly entire elimination of asymmetries in the solution (Figure 1). Table 1 comprises the results of the test. The minimal enhancement of solutions by increasing number of iterations from 2 to 4 is consistent with observations in other tests. Last row of Table 1 summarizes results for the model with *prelimiting* technique. This complementary technique is discussed in Ref. 6. Observe that for free surface environmental flows, long-term transport of sign-preserving properties is typical.

Method	B_{max}	B_{min}	$e(L_\infty)$	$e(L_2)\cdot 10^4$
FEM–CB	0.9194	-0.9098	0.1752	0.2361
NFEM	0.5966	-0.5970	0.4301	0.5796
NFEM 2 iter	0.7482	-0.7479	0.3063	0.4236
NFEM 4 iter	0.7480	-0.7478	0.3035	0.4182
NFEM 2 iter+prelim	0.7482	-0.7479	0.3063	0.4236

Table 1: Sine wave experiment. Results at $12500\Delta t$. Columns indicate: method, maximum value B_{max}, minimum value B_{min}, $e(L_\infty)$: L_∞ error and $e(L_2)$: L_2 error. Δt =0.4.

4 CONCLUDING REMARKS

A sign-preserving continuous finite element method accommodates a low order scheme based on upwinding technique to a high order FEM. This strategy facilitates the use of the procedure by any high order dispersive finite element method, and does not need tuning of artificial diffusion of the low order scheme. In particular, the low order algorithm adds the (nearly) minimum diffusion for positivity. However, classical FCT embedded in the NFEM restricts the portion of accepted high order element contributions. The extension proposed in this work replaces low order solution of NFEM by a predictor solution that satisfies the same requirements. This enhancement permits the desired refinement on the FCT–based approach, while using the most efficient sign-preserving procedure as the predictor first choice.

An iterative procedure with a predictor solution computed by the NFEM put the general correction method into practice. Each iteration reduces the rejected contributions of preceding correction. The method decreases over–diffusion in the corrected solutions and compensates distortions of the FCT in long term smooth problems. The model equipped with an iterative correction has an acceptable extra cost, taking into account that nearly all error reduction is reached after few iterations. In some discontinuous problems, auxiliary tools like prelimiting or *ad hoc* alternative low order schemes are more beneficial than iterative correction to reduce localized ripples due to non–monotonic solutions (see details in Ref. 6).

5 ACKNOWLEDGMENTS

This work was partially supported by the MICIIN grant #BIA-2008-00522. The author is grateful to J.Szmelter and to P.K.Smolarkiewicz for useful discussions.

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