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SOME REMARKS CONCERNING STABILIZATION TECHNIQUES FOR CONVECTION–DIFFUSION PROBLEMS

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Abstract: There are many methods and approaches to solving convection–diffusion problems. For those who want to solve such problems the situation is very confusing and it is very difficult to choose the right method. The aim of this short overview is to provide basic guidelines and to mention the common features of different methods. We place particular emphasis on the concept of linear and non-linear stabilization and its implementation within different approaches.

Keywords: convection, diffusion, stabilization, finite element method, finite volume method, finite difference method

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1. Introduction

Convection and/or diffusion govern several important phenomena in physics and engineering, for example, heat convection and conduction, propagation of pollutants, compressible and incompressible fluid flows (described by the Euler and Navier–Stokes equations). The corresponding equations have fundamentally different properties than the Poisson equation. The convection-dominated phenomena are characterized by skew-symmetric differential operators and solutions of this type of problems contain sharp layers (contact discontinuities, shock waves, boundary layers). The standard finite difference method (FDM), finite volume method (FVM) and Galerkin finite element method (FEM) produce unstable discretizations in the convection-dominated regime. For the Poisson equation, the Galerkin finite element approach minimizes the error in the energy norm. But this is not true for other cases (see [5]). In order to cure these deficiencies, many stabilization techniques have been

proposed with the aim to remove (or to diminish) spurious oscillations without leading to excessive smearing of discontinuities or layers. Numerical solution of the convection–diffusion equations has been the subject of substantial controversy and criticism (see [6]). The problem is still a challenge and much research in this field is needed. It is possible to find formulations as a never-ending story or the 30 years war (see [22] and [10]). This article is a very short and incomplete survey of the techniques used in this field.

The rest of the paper is organized as follows. In Section 2 basic linear methods for problems with slowly varying solutions are presented. Section 3 is devoted to linear methods for problems with rapidly varying solutions. Next, in Section 4, non-linear techniques are discussed. Finally, Section 5 contains concluding remarks.

2. Linear methods for problems with slowly varying solutions

Consider the finite difference method for simple convection problems in the form

$$aq_x = f, \quad q_t + aq_x = f.$$

Here $q = q(x): \mathbb{R} \rightarrow \mathbb{R}$ or $q = q(x, t): \mathbb{R} \times \mathbb{R}_0^+ \rightarrow \mathbb{R}$ is the unknown function we wish to determine, $a \in \mathbb{R}$ is a given constant and $f = f(x): \mathbb{R} \rightarrow \mathbb{R}$ or $f = f(x, t): \mathbb{R} \times \mathbb{R}_0^+ \rightarrow \mathbb{R}$ is a given source of the quantity q . Subscripts are used to denote partial derivatives with respect to x and t . In order to have the classical or weak solution for this problem, the data have to satisfy certain properties that we do not discuss here. To discretize the above equations, we introduce the following notation:

$$\begin{aligned} \Delta x > 0, \quad x_j = j\Delta x, \quad j \in \mathbb{Z}, \quad \Delta t > 0, \quad t_n = n\Delta t, \quad n \in \mathbb{N}_0, \\ Q_j \approx q_j = q(x_j), \quad f_j = f(x_j), \quad Q_j^n \approx q_j^n = q(x_j, t_n), \quad f_j^n = f(x_j, t_n). \end{aligned}$$

Let us first consider two basic schemes for the pure convection problem

$$a \frac{Q_{j+1} - Q_{j-1}}{2\Delta x} = f_j, \quad \frac{Q_j^{n+1} - Q_j^n}{\Delta t} + a \frac{Q_{j+1}^n - Q_{j-1}^n}{2\Delta x} = f_j^n.$$

These schemes are not Lax-Richtmyer stable (linearly stable), i.e., they are not convergent. Moreover, they produce oscillatory solutions. The simplest remedy is to use a one-sided finite difference to approximate the convective term, i.e.,

$$a \frac{Q_j - Q_{j-1}}{\Delta x} = f_j, \quad \frac{Q_j^{n+1} - Q_j^n}{\Delta t} + a \frac{Q_j^n - Q_{j-1}^n}{\Delta x} = f_j^n \quad (\text{if } a > 0). \quad (1)$$

This is the well-known first-order upwind method. In the time-dependent case, it is also possible to apply the Lax–Friedrichs method

$$\frac{Q_j^{n+1} - \frac{1}{2}(Q_{j+1}^n + Q_{j-1}^n)}{\Delta t} + a \frac{Q_{j+1}^n - Q_{j-1}^n}{2\Delta x} = f_j^n, \quad (2)$$

or the Lax–Wendroff method

$$\frac{Q_j^{n+1} - Q_j^n}{\Delta t} + a \frac{Q_{j+1}^n - Q_{j-1}^n}{2\Delta x} - \frac{a^2 \Delta t}{2} \frac{Q_{j+1}^n - 2Q_j^n + Q_{j-1}^n}{(\Delta x)^2} = 0 \quad (\text{if } f = 0).$$

The schemes (1) and (2) can be also rewritten as central schemes with artificial diffusion:

$$\frac{Q_j^{n+1} - Q_j^n}{\Delta t} + a \frac{Q_{j+1}^n - Q_{j-1}^n}{2\Delta x} - \frac{a\Delta x}{2} \frac{Q_{j+1}^n - 2Q_j^n + Q_{j-1}^n}{(\Delta x)^2} = f_j^n,$$

resp.

$$\frac{Q_j^{n+1} - Q_j^n}{\Delta t} + a \frac{Q_{j+1}^n - Q_{j-1}^n}{2\Delta x} - \frac{(\Delta x)^2}{2\Delta t} \frac{Q_{j+1}^n - 2Q_j^n + Q_{j-1}^n}{(\Delta x)^2} = f_j^n.$$

Thus, the above schemes introduce a certain amount of numerical dissipation (diffusion, viscosity). An example of a strictly non-dissipative method is the leapfrog scheme

$$\frac{Q_j^{n+1} - Q_j^{n-1}}{2\Delta t} + a \frac{Q_{j+1}^n - Q_{j-1}^n}{2\Delta x} = f_j^n.$$

Then the numerical solution is not smeared and the scheme is Lax-Richtmyer stable but it leads to a more pronounced dispersion error (caused by the fact that the phase errors are different for different frequencies). Note that a phase error is generally present for any numerical scheme. For more complicated problems it is usually very difficult or even impossible to construct non-dissipative stable schemes. Nevertheless, a certain amount of numerical dissipation may be of advantage since small disturbances in the numerical solution are then damped. Therefore, schemes with numerical dissipation are often preferred.

Alternatives to the schemes (1) are the schemes (again for $a > 0$)

$$a \frac{Q_j - Q_{j-1}}{\Delta x} = \frac{1}{2}(f_{j-1} + f_j), \quad \frac{Q_j^{n+1} - Q_j^n}{\Delta t} + a \frac{Q_j^n - Q_{j-1}^n}{\Delta x} = \frac{1}{2}(f_{j-1}^n + f_j^n), \quad (3)$$

which are motivated by the fact that the steady-state upwind scheme in (3) is second-order accurate.

For the convection–diffusion equations

$$aq_x - bq_{xx} = f, \quad q_t + aq_x - bq_{xx} = f,$$

where $b > 0$ is a given constant, we can use the central schemes

$$a \frac{Q_{j+1} - Q_{j-1}}{2\Delta x} - b \frac{Q_{j+1} - 2Q_j + Q_{j-1}}{(\Delta x)^2} = f_j, \quad (4)$$

resp.

$$\frac{Q_j^{n+1} - Q_j^n}{\Delta t} + a \frac{Q_{j+1}^n - Q_{j-1}^n}{2\Delta x} - b \frac{Q_{j+1}^n - 2Q_j^n + Q_{j-1}^n}{(\Delta x)^2} = f_j^n. \quad (5)$$

The scheme (4) is stable if $|a|\Delta x/2b \leq 1$, i.e., if the approximated solution does not contain boundary layers. This stability condition guarantees the validity of the discrete maximum principle. The scheme (5) is L_2 stable for $b\Delta t/(\Delta x)^2 \leq \frac{1}{2}$. The L_2 stability does not exclude that, for some frequencies, the amplitudes of the numerical solution grow exponentially, which does not correspond to the behaviour of the exact solution. Therefore, one usually requires the scheme to be strongly L_2 stable for which the additional condition $\Delta t \leq 2b/a^2$ is sufficient.

It is also possible to use the standard Galerkin finite element method or the finite volume method. Then we obtain similar stability bounds. The FEM and FVM are more suitable for general cases (complex geometries). The schemes described above and their generalizations are generally suitable for problems with slowly varying solutions, i.e., without layers.

3. Linear methods for problems with rapidly varying solutions

Solutions of problems governed by convection and diffusion may contain boundary and interior layers (convection–diffusion equations, incompressible Navier–Stokes equations), contact discontinuities (pure convection equations), shock waves (non-linear hyperbolic equations like the Burgers equation or Euler equations), shock waves and boundary layers (compressible Navier–Stokes equations). Flows of viscous fluids (described by the Navier–Stokes equations) are often turbulent. Solutions of all the above-mentioned problems are rapidly varying, at least in some regions of the computational domain.

In this section we focus on linear schemes, i.e., schemes that are linear when applied to a linear partial differential equation.

Due to the presence of layers it is useful to introduce different concepts of convergence. One defines the formal accuracy or consistency, i.e., accuracy or consistency for fixed b outside boundary and interior layers. One can also consider uniform convergence (uniform with respect to b) outside interior and boundary layers. Sometimes the concept of uniform convergence (with respect to b) on the whole computational domain is used (see [19]).

For problems with non-smooth and rapidly varying solutions, some numerical stabilization is crucial. The stabilization is added for three distinct purposes (see [15]):

- to eliminate or to suppress high-frequency modes that are not resolved and contaminate the solution;
- to enhance stability and convergence to steady state;
- to prevent oscillations at discontinuities (contact discontinuities, shock waves) or layers.

3.1. Finite difference method

3.1.1. Steady-state case

The standard second-order finite difference scheme (4) described above is based on central differences (for both convection and diffusion terms). This scheme is unstable for convection-dominated case (and unstable in pure convection case). As we mentioned, the stability condition is $|a|\Delta x/2b \leq 1$. Since this condition is often too restrictive, many alternative schemes have been developed. The simplest possibility is to use a one-sided first-order finite difference for the convective term and the central second-order difference for the diffusion term. This leads to a monotonicity preserving scheme which is only of the first order outside layers. One can also use other upwind schemes – these schemes are not generally maximum principle preserving but they are more stable than central schemes. Stoyan (see [21]) proposed a scheme which is second-order accurate outside boundary layers independently of b . This scheme is a generalized version of the Abrahamsson-Keller-Kreiss scheme originating in 1974, see [19]. High-order maximum principle satisfying schemes were proposed, e.g., by Berger et al. (see [2]). Uniformly convergent methods were also proposed, e.g., the Il'in-Allen-Southwell scheme which is of the second order for fixed b and first-order uniformly convergent on the whole domain (see [19]). There are also uniformly convergent methods based on non-uniform meshes, in particular, on graded and piecewise equidistant meshes (Bakhvalov, Shishkin) (see [19]).

3.1.2. Evolutionary case

The finite difference scheme (5) satisfies the discrete maximum principle if $|a|\Delta x/2b \leq 1$ and $\Delta t \leq (\Delta x)^2/2b$. These conditions often require very fine meshes and small time steps. As a remedy, an upwind discretization of the convection term can be again applied. The resulting method is stable and first-order accurate. High-order methods are L_2 stable but can produce oscillatory numerical results (we recall the well known Godunov barrier theorem for the convection case). In case of linear convection with a constant coefficient it is possible to combine the Lax-Wendroff and Beam-Warming method to obtain a third-order L_∞ stable method. Note that odd-order schemes are usually preferred, e.g., Leonard QUICKEST (Quadratic Upstream Interpolation for Convective Kinematics with Estimated Streaming Terms) scheme, see [13], because the leading error term contains an even order derivative (i.e., the leading error term is dissipative, see [4]).

3.2. Finite volume method

3.2.1. Steady-state case

Finite volume methods stem from integral conservation or balance relations over a control volume. They are based on the approximation of fluxes (the approximations are called numerical fluxes). These techniques are very often used in computational fluid dynamics. They preserve the conservation property on the discrete level (up to machine precision). There are many finite volume schemes, e.g., schemes based

on central numerical fluxes, upwind fluxes (these schemes lead to standard finite difference schemes on uniform meshes) or the Il'in-Allen-Southwell scheme called Scharfetter-Gummel scheme. The benefits of the finite volume method are more pronounced in 2D and 3D cases.

3.2.2. Evolutionary case

It is very useful to formulate the finite volume method for the evolutionary case in the RSA fashion (Reconstruct - Solve - Average, see [14]):

- R** Reconstruct a (piecewise polynomial) function defined for all x , from the cell averages.
- S** Solve the convection part of the equation exactly (or approximately) with this initial data to obtain a solution on the next time level (i.e., solve the so-called Riemann problems). This solution is used to compute numerical fluxes. Compute the numerical viscous fluxes.
- A** Average the solutions of the Riemann problems over each grid cell to obtain new cell averages (or use the numerical fluxes to compute the cell averages).

One obtains different schemes depending on the reconstruction technique, Riemann solver and numerical fluxes. In the 1D case the derived schemes are analogous to the finite difference schemes. Riemann solvers are an efficient tool to evolve non-smooth data between time steps (or to evolve unresolved fine scales for given coarse scale data, see [23]). But we have also to mention the great Riemann solver debate – the discussion devoted to the drawbacks of the methods based on 1D Riemann solvers.

3.3. Finite element method

In the 1D case, the standard Galerkin finite element method based on continuous piecewise linear approximation on an equidistant mesh generates the central finite difference scheme (4) for constant data. Many types of stabilized finite element methods of upwind type have been developed. For example, one can switch to a Petrov-Galerkin method with asymmetric basis functions in the test function space or one can use the finite volume idea to discretize the convective term. This method is stable and of the first order (i.e., the formal order is equal to 1). Many other stabilized finite element methods were developed by adding further terms to the variational formulation.

3.3.1. SUPG method (SDFEM)

Consider the steady-state convection–diffusion–reaction problem

$$-bq_{xx} + aq_x + cq = f \quad \text{in } (0, 1), \quad u(0) = u(1) = 0,$$

where, for simplicity, the coefficients a , b , and c are constant and $f \in L_2(0,1)$. Moreover, $b > 0$. The weak solution q belongs to the space $V = H_0^1(0,1)$ and satisfies the variational formulation

$$A(q, v) = F(v) \quad \forall v \in V,$$

where $A(q, v) = b(q_x, v_x) + (aq_x + cq, v)$, $F(v) = (f, v)$, with (\cdot, \cdot) denoting the inner product in the space $L_2(0,1)$.

Now we apply the finite element method. We divide the interval $(0,1)$ into M subintervals of equal length h and denote the corresponding nodes by $x_j = jh$, $j = 0, 1, \dots, M$. Let $V_h \subset V$ be the space of continuous piecewise polynomial functions on this mesh. Then the Galerkin FEM defines a numerical solution $q_h \in V_h$ satisfying

$$A(q_h, v_h) = F(v_h) \quad \forall v_h \in V_h.$$

If V_h consists of piecewise linear functions, then this approach generates a central finite difference scheme (if $c = 0$, it is the scheme (4) with $\Delta x = h$ and $Q_j = q_h(x_j)$). Hence the Galerkin method is not appropriate in the convection-dominated regime. A possible remedy is to use the Streamline Upwind/Petrov-Galerkin (SUPG) method, also called Streamline Diffusion FEM (SDFEM): find $q_h \in V_h$ such that

$$A_h(q_h, v_h) = F_h(v_h) \quad \forall v_h \in V_h,$$

where

$$A_h(q, v) = A(q, v) + \sum_{i=1}^M \int_{x_{i-1}}^{x_i} (-bq_{xx} + aq_x + cq) \delta_h a v_x \, dx,$$

$$F_h(v) = F(v) + (f, \delta_h a v_x),$$

and δ_h is a non-negative stabilization parameter. This approach is frequently used since it combines good stability properties with a high accuracy outside the layers. In particular, this method is consistent, i.e., the exact solution satisfies $A_h(q, v_h) = F_h(v_h)$ for any $v_h \in V_h$.

The order of the method depends on the choice of the artificial diffusion (i.e., on the choice of δ_h) and on the degree of polynomials used for defining the space V_h . The stabilization parameter δ_h depends on the Péclet number $Pe = |a|h/2b$ and can be chosen, e.g., as follows (see [19])

$$\delta_h = \begin{cases} C_1 \frac{h^2}{b} & \text{for } Pe < 1, \\ C_2 \frac{h}{|a|} & \text{for } Pe \geq 1, \end{cases} \quad \delta_h = \frac{h}{2|a|} \left(\coth Pe - \frac{1}{Pe} \right).$$

The second choice leads to a uniformly convergent method. There are many other linear stabilization techniques, e.g., VMS (Variational Multiscale Method), DRM

(Differentiated Residual Method), RFB (Residual Free Bubbles), DEM (Discontinuous Enrichment Method), CIP (Continuous Interior Penalty), GLS (Galerkin Least Squares), LPS (Local Projection Stabilization), see [19], [8], [20].

3.3.2. Finite element method – evolutionary case

In the evolutionary case the solution may also have one or more interior layers (caused by the initial and boundary conditions). The methods described in the previous section can be applied. We can use, e.g., the Euler or Crank–Nicolson scheme to discretize the time derivative. In case of residual-based methods the choice of the stabilization parameter is more complicated (the convective term is combined, i.e., it has the form $q_t + aq_x$). The stabilization parameter depends on the time step. More suitable choices seem to be the CIP or LPS approaches.

3.3.3. DGFEM (Discontinuous Galerkin FEM)

This method is a combination of the Galerkin FEM and the Riemann solver based approach applied to discontinuous piecewise polynomial approximations. The first version of the method was formulated by Reed and Hill to solve the particle transport problem (see [16]). The first-order version of DGFEM is identical to the finite volume Godunov scheme (or more precisely to the version with the local Lax–Friedrichs numerical flux). The stabilization procedure is implemented through the numerical fluxes. There are many versions of the DGFEM both for steady-state and evolutionary cases. The main advantages of the DGFEM are flexibility with respect to the mesh, simple hp -adaptivity, and simple treatment of convective terms and boundary conditions (see [19]). The method is also efficiently parallelizable. The main disadvantage is that the number of degrees of freedom is larger than the number of degrees of freedom in the case of FDM, FVM or FEM.

4. Non-linear methods for problems with rapidly varying solutions

In most cases, to remove or sufficiently suppress spurious oscillations without introducing too much artificial diffusion, non-linear stabilizations have to be used. There are many non-linear methods that have different properties: TVD (Total Variation Diminishing), TVB (Total Variation Bounded), LED (Local Extremum Diminishing), monotone or monotonicity preserving. The methods are well understood in the 1D case, but in several spatial dimensions the situation is much more complicated. For example, it is proven that TVD methods are at most of second order in 1D and at most of first order in the multi-dimensional evolutionary case. Development of high-order methods (i.e., methods that are of third or higher order) for systems of equations in the multi-dimensional case is a very complex task, also due to the fact that we do not have a sufficient theoretical background.

4.1. Non-linear stabilization techniques

There are different techniques for non-linear stabilization (developed originally for FDM and FVM, see [7], [17]):

- Slope limiter methods based on the RSA approach that is described above. Non-linear stabilization is realized through the reconstruction with limiters or (W)ENO (Weighted Essentially Non-Oscillatory) reconstruction. This approach is suitable together with the discontinuous approximation and can be combined with (approximate) Riemann solvers.
- Flux limiter methods based on combining any low-order numerical flux and any higher-order numerical flux. This approach appeared in the hybrid method of Harten and Zwas and the FCT (Flux-Corrected Transport) method of Boris and Book (see [3]).
- Artificial viscosity approach based on the von Neumann idea. This idea was further developed by a number of authors in various forms.

However, the use of these procedures is not always straightforward and simple. Unfortunately, some of the above mentioned procedures are not free of parameter tuning.

4.2. Non-linear stabilizations in the finite element method

As we already mentioned, linear methods of higher order are not monotone, which causes that numerical solutions are often polluted by spurious oscillations. Therefore, various non-linear stabilizations have been proposed which are known as shock capturing methods, discontinuity capturing methods or spurious oscillations at layers diminishing (SOLD) methods, see [9] for a review of approaches for steady-state convection–diffusion equations. The aim of these approaches is to reduce or remove spurious oscillations by adding an additional artificial diffusion term to a linear stabilization method. The amount of this artificial diffusion depends on the unknown numerical solution so that the resulting method is non-linear. The additional term usually represents either isotropic or crosswind (i.e., orthogonal to the convection direction) artificial diffusion, however, also approaches based on edge stabilization or of LPS type can be found in the literature. For non-linear stabilizations, there are considerably less theoretical results available than for linear methods; in some cases, the solvability, error estimates or the validity of the discrete maximum principle were proved.

Although the non-linear stabilizations often significantly improve solutions of linear stabilization methods, they are generally not able to remove the spurious oscillations completely. The only exceptions are methods satisfying the discrete maximum principle which, however, usually lead to an unacceptable smearing of the numerical solution. Some of the methods involve parameters which may be adjusted to improve the quality of the solution. Unfortunately, it turns out, that these parameters are non-constant in general and depend on the data and the grid so that it is not clear how to choose them for more complicated problems in advance. A possible remedy is to optimize the parameters in an automatic way by minimizing a suitable target functional (see [11]). In this way, also the solutions provided by linear stabilization methods can be significantly improved.

A possible criticism of non-linear stabilizations stems from the fact that the solution of the non-linear algebraic problems is often quite expensive in comparison with the solution of linear problems. Nevertheless, most of the applications in which convection dominates are modeled by non-linear partial differential equations and then the use of a non-linear stabilization does not constitute a significant overhead. In any case, the solution of non-linear algebraic problems requires the choice of appropriate numerical approaches and it is not always easy to achieve a convergence of the used solver.

4.3. Algebraic stabilization

There are many strategies to implement non-linear stabilizations of finite difference and finite volume methods (TVD, ENO, WENO, LED, FCT). In the case of the Galerkin FEM the most common strategies are based on a modification of the variational formulation or on enrichment the finite-dimensional basis. AFC (Algebraic Flux Correction) is an alternative approach that acts on the algebraic level, i.e., on the level of discrete operators. The basic approach is an analogy of the FCT scheme. For suitable limiter functions the AFC schemes satisfy the discrete maximum principle and linearity preservation on arbitrary meshes (see [12] and [1]). This implies the preservation of second-order accuracy in smooth regions.

4.4. Multi-dimensional evolutionary problems

The Godunov-type finite-volume methods and their successors (which include discontinuous Galerkin and (W)ENO schemes) are based on one-dimensional (approximate) Riemann solvers. But it is very difficult, if not impossible, to find a solution to the multi-dimensional Riemann problem. We already mentioned several times that no numerical method, even for linear scalar convection equation, can be both monotone and better than first-order accurate. Instead of too complicated high-order methods based on the multi-dimensional Riemann solvers, a number of alternative approaches have been developed based on the continuous approximation of the solution (see [18]). These approaches are Riemann solver-free. It is possible to construct their non-linear versions that are of higher order. Such methods include, e.g., RDS (Residual Distribution Schemes) based on the fluctuation splitting proposed by Roe and Active Flux Schemes. Flux Vector Splitting schemes and kinetic Boltzmann approach can also be used.

5. Conclusions

Linear stabilization can be accomplished by many techniques. Because of the Godunov barrier theorem it is not possible to construct linear monotonicity preserving schemes that are of higher (formal) order than 1 in the evolutionary convection case. In the convection–diffusion case it seems that, in general, linear stabilizations are able only to suppress spurious oscillations if layers should not be smeared too much. The discontinuous approximation and Riemann based approach are not sufficient for

a complete elimination of unphysical wiggles. However, these two algorithm components play a very important role: the first component allows or simplifies stable (constrained) L_2 projection (averaging, reconstruction or limiting) and the second one evolves unresolved fine scales. On the other hand, approximate Riemann solvers or upwind techniques (partially based on wave averaging instead of wave evolving) combined with averaging, reconstruction or L_2 projection usually introduce a non-negligible amount of the artificial dissipation.

To obtain higher-order monotonicity preserving schemes, non-linear discretizations have to be applied. There are also many non-linear approaches that are not monotonicity preserving but considerably reduce spurious oscillations. The non-linear techniques are of advantage also for first-order methods since they add artificial diffusion only in regions where it is required by the character of the solution (in particular, in regions of layers, discontinuities and extrema) so that the resulting approximate solutions do not suffer from excessive smearing. A drawback of these methods may be the increased computational cost connected with the numerical solution of the non-linear algebraic systems. However, when these techniques are applied to non-linear problems, this issue is often of minor importance.

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